8-1008

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner # : 59193 Date: 8/22/06

Art Unit: 1624 Phone Number: 2- 0663 Serial Number: 10608689

Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): (PAPER) DISK

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To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: _____

Inventors (please provide full names): _____

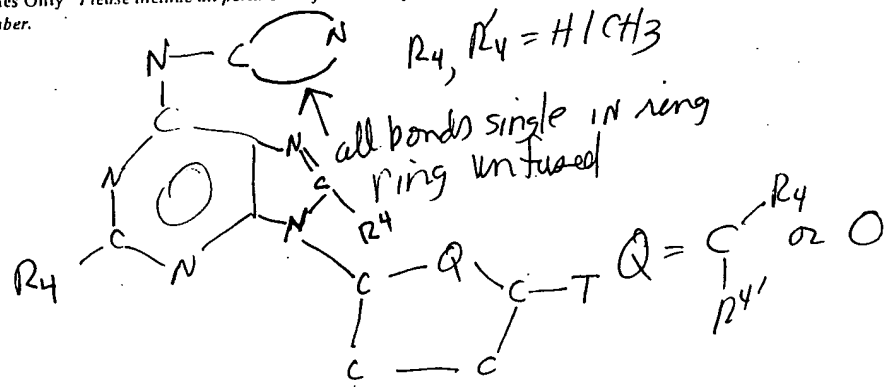
_____

Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



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STAFF USE ONLY

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Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: 8/24/06

Date Completed: 8/24/06

Searcher Prep & Review Time: 30

Online Time: 60

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

3 Structure (#)

_____ Bibliographic

_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

$274.0 STN _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

____ In-house sequence systems

____ Commercial ____ Oligomer ____ Score/Length

____ Interference ____ SPDI ____ Encode/Transl

_____ Other (specify)

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                 SEL RN

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L18           28 S L2 NOT L17
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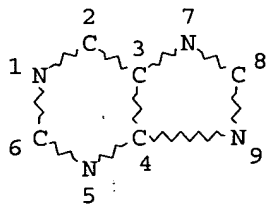


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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
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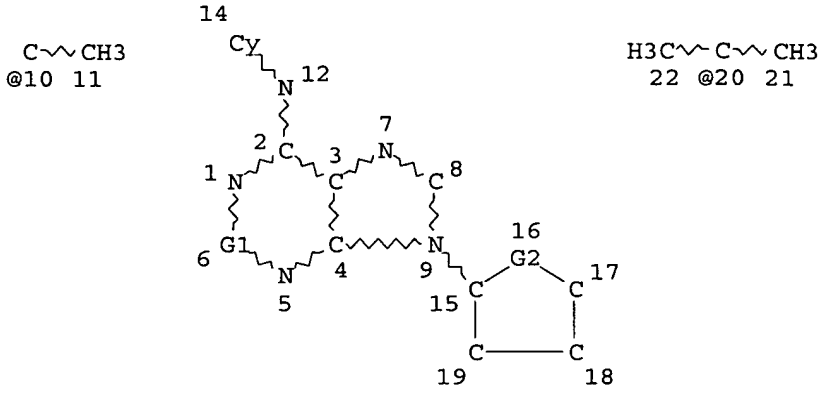

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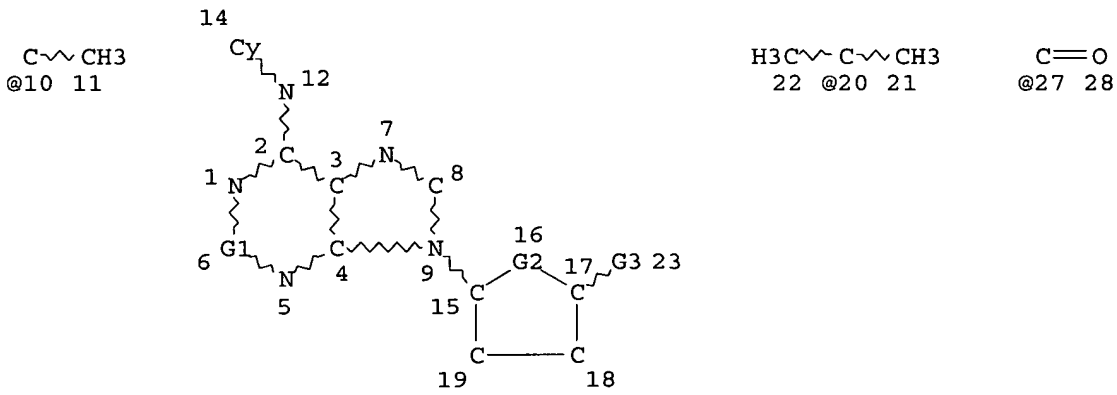

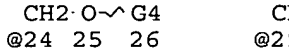

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FILE 'HCAPLUS' ENTERED AT 10:57:53 ON 24 AUG 2006

=> d l22 1-35 ibib abs hitstr hitind

L22  ANSWER 1 OF 35  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2006:337894  HCAPLUS
DOCUMENT NUMBER:          144:384968
TITLE:                    Engineered protein kinases which can utilize
                          modified nucleotide triphosphate substrates
INVENTOR(S):              Shokat, Kevan
PATENT ASSIGNEE(S):       Princeton University, USA
SOURCE:                   U.S., 54 pp., Cont.-in-part of U.S. Ser. No.
                          797,522.
                          CODEN: USXXAM
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     US 7026461            B1    20060411    US 2001-985061
                                                                    2001
                                                                    1101
     WO 9835048            A2    19980813    WO 1998-US2522
                                                                    1998
                                                                    0209
     WO 9835048            A3    19990107
         W:  AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GW, HU,
             ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN,
             MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ,
             VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK,
             ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
     EP 1607481            A1    20051221    EP 2004-76255
                                                                    1998
                                                                    0209
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
             MC, PT, IE, FI
     JP 2004248675         A2    20040909    JP 2004-87151
                                                                    2004
                                                                    0324
PRIORITY APPLN. INFO.:                       US 1997-797522      B2
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1997
0207

US 1997-46727P P
1997
0516

WO 1998-US2522 W
1998
0209

US 1999-367065 A3
1999
1117

EP 1998-906268 A3
1998
0209

JP 1998-534999 A3
1998
0209

AB The present invention involves the engineering of kinases and other multi-substrate enzymes such that they can become bound by inhibitors which are not as readily bound by their wild-type forms. In a first aspect, the present invention involves the engineering of kinases and other multi-substrate enzymes such that they can utilize modified substrates which are not as readily used by their wildtype forms. The invention further provides such chemical modified nucleotide triphosphate substrates, methods of making them, and methods of using them. The methods of the present invention include methods for using the modified substrates along with the engineered kinases to identify which protein substrates the kinases act upon, to measure the extent of such action, and to determine if test compds. can modulate such action. An engineered kinase made according to the present invention will be able to use an orthogonal nucleotide triphosphate substrate that is not as readily used by other, non-engineered kinases present in cells. By labeling the phosphate on the orthogonal substrate, e.g., by using radioactive phosphorous (p32), and then adding that labeled substrate to permeabilized cells or cell exts., the protein substrates of the engineered kinase will become labeled, whereas the protein substrates of other kinases will be at least labeled to a lesser degree; preferably, the protein substrates of the other kinases will not be substantially labeled, and most preferably, they will not be labeled at all. The detailed description and examples provided below describe the use of this strategy to uniquely tag the direct substrates of the prototypical tyrosine kinase, v-Src. Through protein engineering a chemical difference has been made in the amino acid sequence which imparts a new structural distinction between the nucleotide binding site of the modified v-Src and that of all other kinases. The v-Src kinase the inventors have engineered recognizes an ATP analog (A*TP), N6-(cyclopentyl)ATP, which is orthogonal to the nucleotide substrate of wild-type kinases. The generation of a v-Src mutant with specificity for an orthogonal A*TP substrate allows for the direct substrates of v-Src to be uniquely radiolabeled using (γ-32P) N6-(cyclopentyl)ATP, because it is able to serve as substrate to the engineered v-Src kinase, but

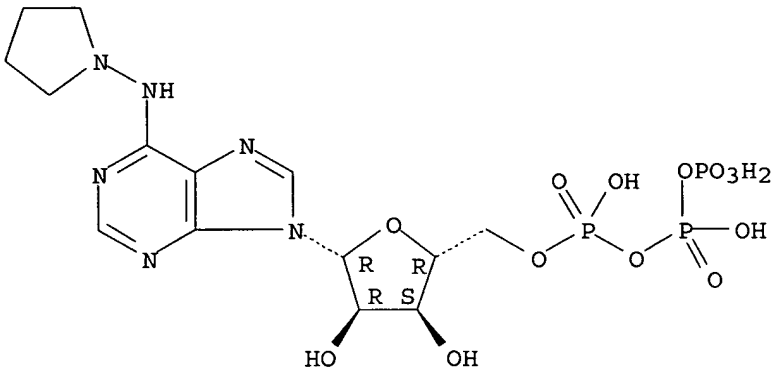
is not substantially able to serve as substrate for other cellular kinases. The detailed description and examples provided below describe the use of this strategy to uniquely identify the direct substrates of the prototypical tyrosine kinase, v-Src. The engineered v-Src kinases that have been made and presented herein bind to an orthogonal analog of the more general kinase inhibitor PP3: the compound N04 cyclopentoyl PP3. The generation of a v-Src mutant with specificity for such an inhibitor allows for the mutant to be inhibited, whereas other kinases in the same test system are not substantially inhibited, not even the wildtype form of that same kinase.

IT **882299-27-6**, N6-(Pyrolidino)ATP **882299-28-7**, N6-(Piperidino)ATP
(engineered protein kinases which can utilize modified nucleotide triphosphate substrates)

RN 882299-27-6 HCAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), N-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

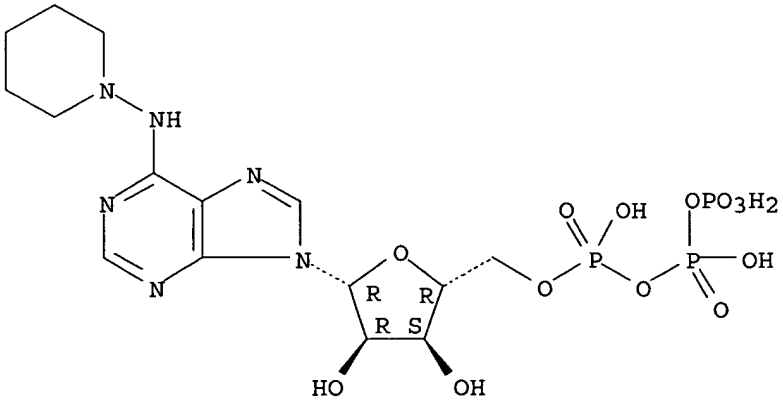
Absolute stereochemistry.



RN 882299-28-7 HCAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), N-1-piperidinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



INCL 536023100; 536023200; 536023600; 536023700; 536024310; 536024500; 536024320; 536024330; 514013000; 514014000

CC 7-8 (Enzymes)
Section cross-reference(s): 9, 33
IT 40922-97-2, N6-(Benzyl)ATP 55296-60-1, N6(Methoxy)ATP
189822-11-5, N6-(Cyclopentyl)ATP 206978-65-6, N6(Ethoxy)ATP
206978-66-7, N6(Acetyl)ATP 206978-67-8, N6(Isopropoxy)ATP
206978-68-9, N6-(Benzyloxy)ATP 206978-70-3, N6-(Cyclopentyloxy)ATP 206978-73-6, N6-(Cyclohexyl)ATP
206978-74-7, N6-(Cyclohexyloxy)ATP **882299-27-6**,
N6-(Pyrolidino)ATP **882299-28-7**, N6-(Piperidino)ATP
(engineered protein kinases which can utilize modified nucleotide triphosphate substrates)
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:267347 HCAPLUS
DOCUMENT NUMBER: 140:271150
TITLE: Preparation of acetylene nucleosides as therapeutic adenosine A1 receptor agonists
INVENTOR(S): Ellis, Frank; Fulton, Heather Elizabeth; Hall, Adrian; Jaxa-Chamiec, Albert Andrzej; Swanson, Stephen; Vile, Sadie
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026890	A1	20040401	WO 2003-EP10350	2003 0916
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003260509	A1	20040408	AU 2003-260509	2003 0916

PRIORITY APPLN. INFO.:	GB 2002-21694	A	2002 0918
	WO 2003-EP10350	W	2003 0916

OTHER SOURCE(S): MARPAT 140:271150
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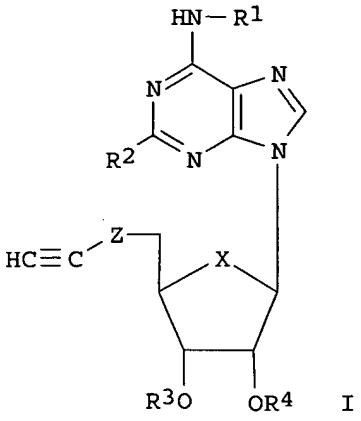


I

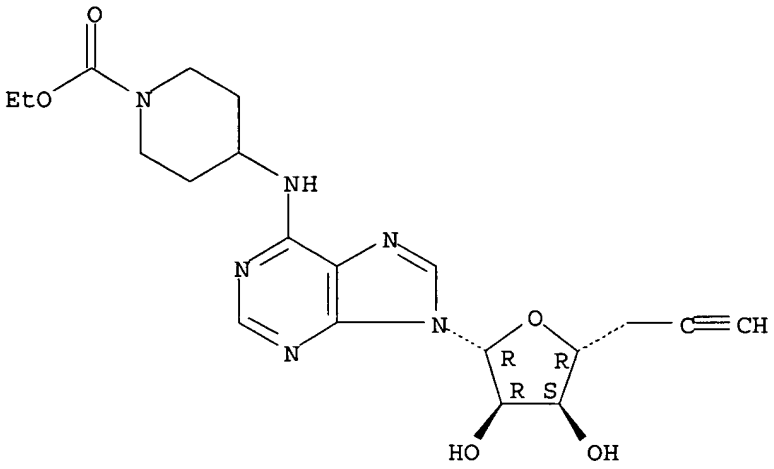
AB Acetylene nucleosides I, wherein wherein X represents O or CH2; Z represents (CH2)p or (CH2OCH2) wherein p = 1-3; R1 represents substituted alkylenecycloalkyl, alkylenecycloalkenyl, substituted Ph, heterocycle, alkyl; R2 represents alkyl, halogen, hydrogen or alkoxy group; R3 and R4 are independently hydrogen or alkyl group; were prepared as are adenosine A1 agonists, and used in therapy. Thus, (2R,3R,4S,5R)-2-[6-(2,2-dimethylcyclopropylamino)purin-9-yl]-5-prop-2-ynyloxymethyltetrahydrofuran-3,4-diol was prepared and used as therapeutic adenosine A1 receptor agonist. Title nucleosides are used as medicament for the treatment of a patient suffering from or susceptible to ischemic heart disease, peripheral vascular disease or stroke or which subject is suffering pain, a CNS disorder, sleep apnea or emesis.

IT **674367-64-7P**
(preparation of acetylene nucleosides as therapeutic adenosine receptor agonists)

RN 674367-64-7 HCAPLUS

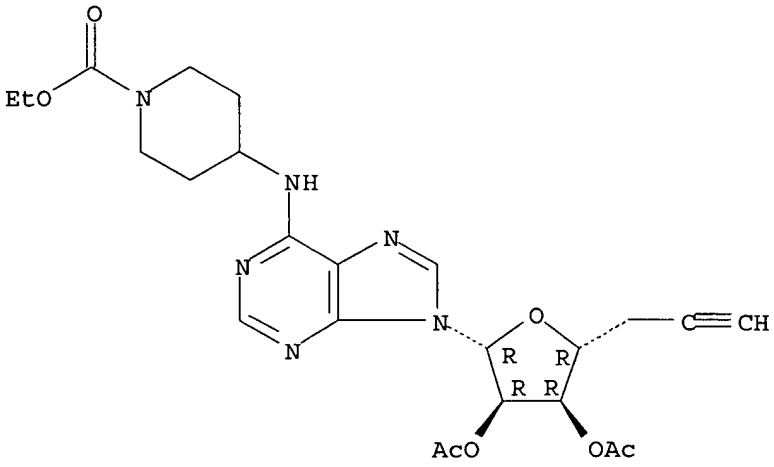
CN 1-Piperidinecarboxylic acid, 4-[[9-(5,6,7-trideoxy-β-D-ribo-hept-6-ynofuranosyl)-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **674367-59-0P**
(preparation of acetylene nucleosides as therapeutic adenosine receptor agonists)
RN 674367-59-0 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[2,3-di-O-acetyl-5,6,7-trideoxy-β-D-ribo-hept-6-ynofuranosyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS C07D473-18; C07D473-34; A61K031-70; A61P009-10
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT 674367-35-2P 674367-36-3P 674367-37-4P 674367-38-5P
674367-39-6P 674367-42-1P 674367-44-3P 674367-45-4P
674367-46-5P 674367-47-6P 674367-48-7P 674367-49-8P
674367-50-1P 674367-51-2P 674367-61-4P 674367-62-5P
674367-63-6P **674367-64-7P** 674799-98-5P
(preparation of acetylene nucleosides as therapeutic adenosine receptor agonists)

IT 674367-26-1P 674367-27-2P 674367-30-7P 674367-31-8P
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674367-43-2P 674367-52-3P 674367-53-4P 674367-54-5P
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674367-59-0P 674367-60-3P 674799-97-4P
(preparation of acetylene nucleosides as therapeutic adenosine receptor agonists)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:5177 HCAPLUS
DOCUMENT NUMBER: 140:42425
TITLE: Preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes
INVENTOR(S): Bigot, Antony; Stengelin, Siegfried; Jaehne, Gerhard; Herling, Andreas; Mueller, Guenter; Hock, Franz Jakob; Myers, Michael R.
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1375508	A1	20040102	EP 2002-14324	20020627
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CA 2490253	AA	20040108	CA 2003-2490253	20030626
WO 2004003002	A1	20040108	WO 2003-EP6749	20030626
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AU 2003280141	A1	20040119	AU 2003-280141	20030626
BR 2003012428	A	20050426	BR 2003-12428	20030626

EP 1527083	A1	20050504	EP 2003-740352	2003 0626
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CN 1671728	A	20050921	CN 2003-817966	2003 0626
JP 2006501178	T2	20060112	JP 2004-516688	2003 0626
US 2004127434	A1	20040701	US 2003-608689	2003 0627
NO 2005000398	A	20050125	NO 2005-398	2005 0125
PRIORITY APPLN. INFO.:			EP 2002-14324 A	2002 0627
			US 2002-434164P P	2002 1217
			WO 2003-EP6749 W	2003 0626

OTHER SOURCE(S): MARPAT 140:42425

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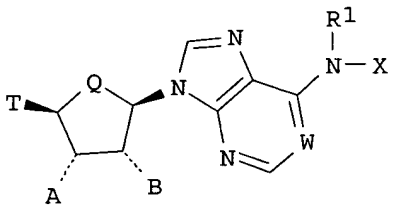


I

AB Adenosine analogs I, wherein W is N, NO, CH; Q is CH2, O; R1 is alkyl, allyl, 2-methylallyl, 2-butenyl, cycloalkyl; X is heterocycle; T is cycloalkyl, aryl-(alkylene)-, heterocyclyl-(alkylene), which residues are monosubstituted by halogen or OR2, halogen, pseudo-halogen, mercapto, NH2, nitro, hydroxy, unsubstituted and at least monosubstituted alkyl, alkoxy, (alkyl)amino, (alkyl)thio, aryl and heterocyclyl; R2 is alkyl substituted by at least one halogen; A and B are independently H, alkyl, hydroxy-(alkylene)-, alkoxy-(alkylene)-, or OR'; R' is hydrogen, alkyl, aryl-(alkylene)-, (alkyl)-CO, carbo-alkoxy, aryl-(alkylene)-CO-, and aryl-O-CO-; were prepared for the treatment of insulin resistance syndrome and diabetes. These compds. are useful for the manufacture of a medicament for the treatment of insulin resistance, type 2 diabetes, metabolic syndrome, lipid disorders or cardiovascular disease or for providing an anti-lipolytic

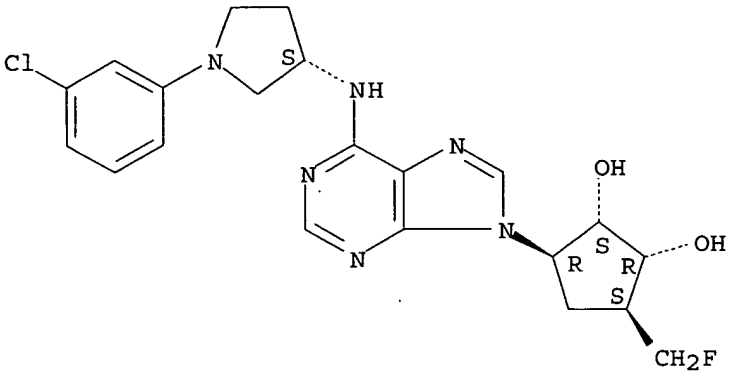
effect. Thus, (1R,2S,3R,5S)-3-{6-[1-(3-chloro-phenyl-1-yl)-pyrrolidin-3(S)-ylamino]-purin-9-yl}-5-fluoromethylcyclopentane-1,2-diol was prepared and used in vitro or the treatment of insulin resistance syndrome and diabetes. Measurement of insulin sensitivity in conscious insulin resistant Zucker fatty rats or Zucker diabetic fatty (ZDF) rats is reported. Effect of title nucleosides on contractile force and heart rate, is reported.

IT **636600-26-5P 636600-34-5P 636600-35-6P 636600-36-7P**
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)

RN 636600-26-5 HCAPLUS

CN 1,2-Cyclopentanediol, 3-[6-[[(3S)-1-(3-chlorophenyl)-3-pyrrolidinyl]amino]-9H-purin-9-yl]-5-(fluoromethyl)-, (1R,2S,3R,5S)- (9CI) (CA INDEX NAME)

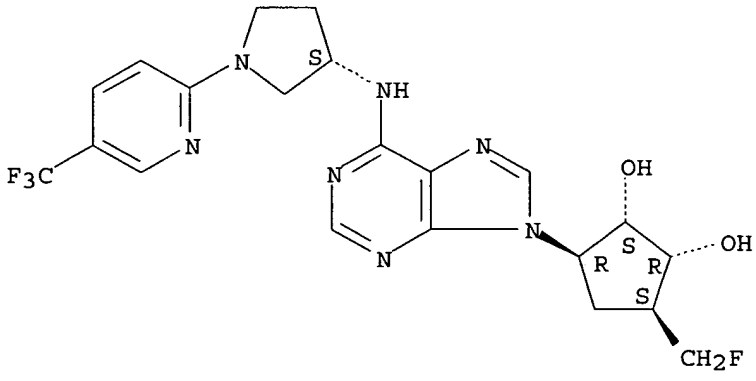
Absolute stereochemistry.



RN 636600-34-5 HCAPLUS

CN 1,2-Cyclopentanediol, 3-(fluoromethyl)-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)- (9CI) (CA INDEX NAME)

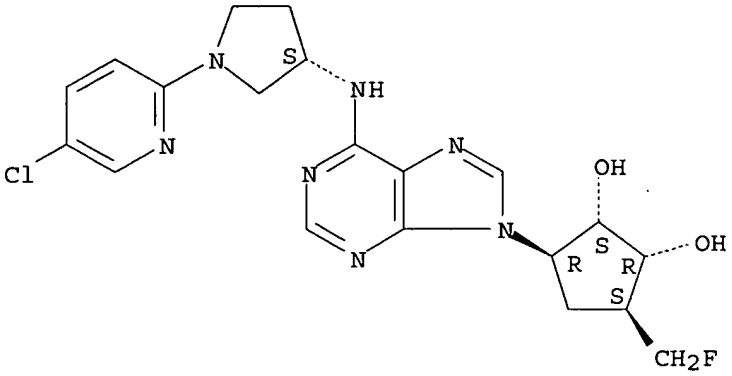
Absolute stereochemistry.



RN 636600-35-6 HCAPLUS

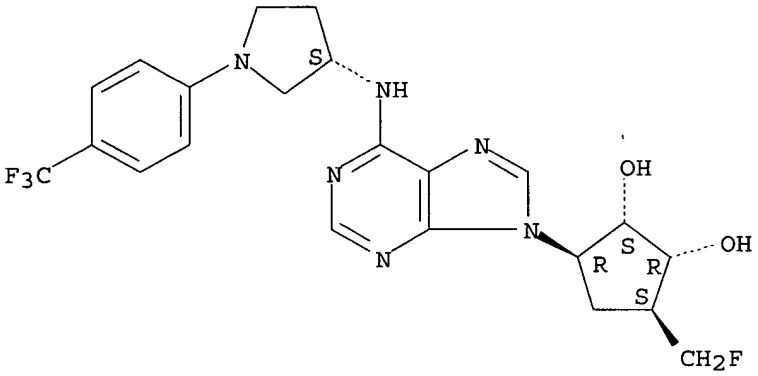
CN 1,2-Cyclopentanediol, 3-[6-[[(3S)-1-(5-chloro-2-pyridinyl)-3-pyrrolidinyl]amino]-9H-purin-9-yl]-5-(fluoromethyl)-, (1R,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 636600-36-7 HCAPLUS
CN 1,2-Cyclopentanediol, 3-(fluoromethyl)-5-[6-[[(3S)-1-[4-(trifluoromethyl)phenyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-167
ICS A61K031-70
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT **636600-26-5P** 636600-28-7P 636600-31-2P
636600-34-5P 636600-35-6P 636600-36-7P
636600-37-8P 636600-38-9P 636600-39-0P 636600-40-3P
636600-41-4P 636600-42-5P 636600-43-6P 636600-44-7P
636600-45-8P 636600-46-9P 636600-47-0P
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:885976 HCAPLUS
DOCUMENT NUMBER: 137:370321
TITLE: Preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes

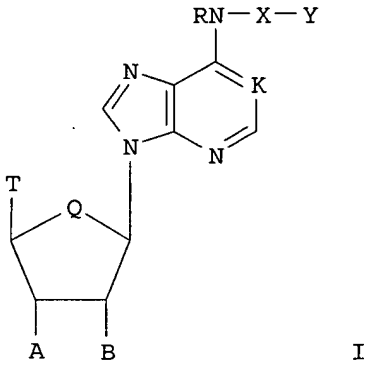
INVENTOR(S): Herling, Andreas; Jaehne, Gerhard; Maguire, Martin P.; Spada, Alfred P.; Myers, Michael R.; Choi-Sledeski, Yong Mi; Pauls, Heinz W.; Ewing, William R.
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: Eur. Pat. Appl., 41 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1258247	A1	20021120	EP 2001-111651	2001 0514
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CA 2447408	AA	20021121	CA 2002-2447408	2002 0514
WO 2002092093	A1	20021121	WO 2002-EP5301	2002 0514
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003176390	A1	20030918	US 2002-145207	2002 0514
EE 200300551	A	20040216	EE 2003-551	2002 0514
EP 1404338	A1	20040407	EP 2002-769485	2002 0514
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002009650	A	20040713	BR 2002-9650	2002 0514
CN 1518450	A	20040804	CN 2002-811239	2002 0514
JP 2004533448	T2	20041104	JP 2002-589010	2002 0514
NZ 529390	A	20060630	NZ 2002-529390	2002 0514

BG 108356	A	20041230	BG 2003-108356	2003 1113
PRIORITY APPLN. INFO.:			EP 2001-111651	A 2001 0514
			WO 2002-EP5301	W 2002 0514

OTHER SOURCE(S): MARPAT 137:370321

GI



I

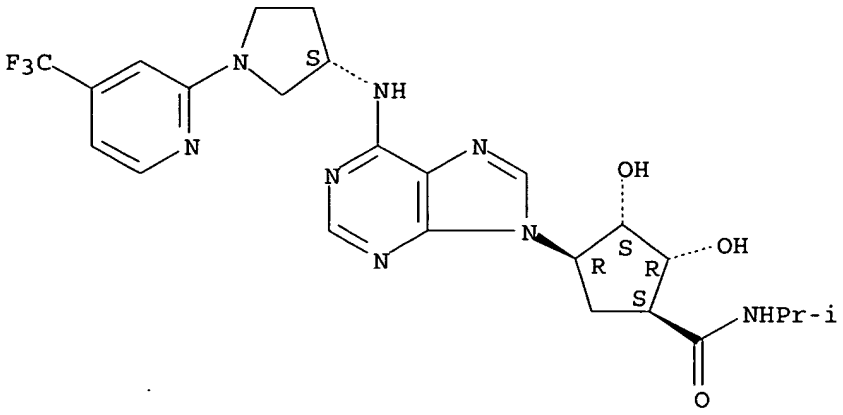
AB The invention relates to the use of adenosine compds. I wherein K is N, N→O, or CH; Q is CH2 or O; R is hydrogen, alkyl, allyl, 2-methallyl, 2-butenyl, cycloalkyl; X is N-containing heterocycle; E is O or S; Y is hydrogen, alkyl, aralkyl, aryl; T is hydrogen, alkyl, acyl, thioacyl, halo, carboxyl; amide, thioamide; A and B are independently is hydrogen, OH, alkyl, hydroxyalkyl, alkoxy, alkoxyalkyl, and certain derivs. thereof for producing a medicine for the treatment of the insulin resistance syndrome and diabetes. Thus, (2R,3R,4S,5R)-2-hydroxymethyl-5-[6-[1-(5-chloropyridin-2-yl)-pyrrolidin-3(S)-ylamino]-purin-9-yl]-tetrahydrofuran-3,4-diol was prepared for the treatment of insulin resistance syndrome and diabetes. Measurement of insulin sensitivity in conscious rats and in vitro adenosine receptor binding affinity determination were reported.

IT **202267-01-4P 202267-53-6P 202267-83-2P 202267-84-3P 475290-54-1P**
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)

RN 202267-01-4 HCAPLUS

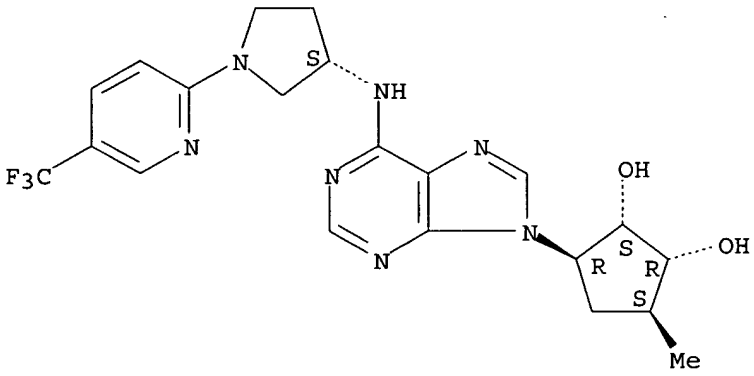
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-(1-methylethyl)-4-[6-[[(3S)-1-[4-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



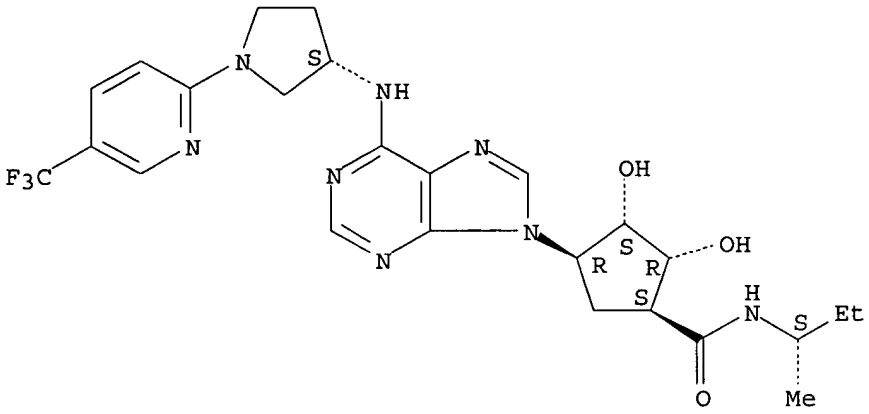
RN 202267-53-6 HCAPLUS
CN 1,2-Cyclopentanediol, 3-methyl-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



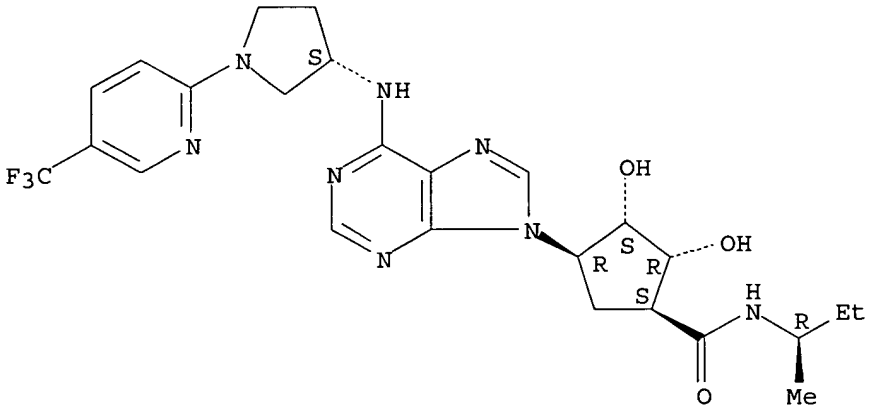
RN 202267-83-2 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1S)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



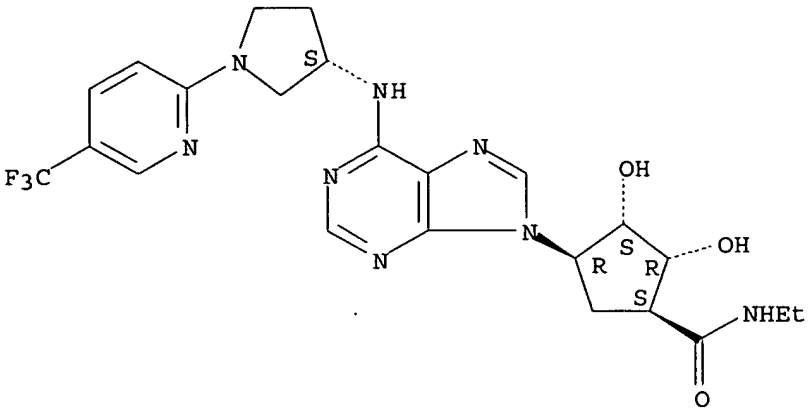
RN 202267-84-3 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1R)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 475290-54-1 HCAPLUS
CN Cyclopentanecarboxamide, N-ethyl-2,3-dihydroxy-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-52
ICS A61P003-10
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT **202267-01-4P** 202267-06-9P 202267-14-9P 202267-16-1P
202267-20-7P 202267-30-9P 202267-31-0P 202267-32-1P
202267-33-2P 202267-34-3P 202267-36-5P 202267-37-6P
202267-39-8P 202267-40-1P 202267-41-2P 202267-42-3P
202267-43-4P 202267-45-6P 202267-48-9P 202267-49-0P
202267-50-3P 202267-51-4P **202267-53-6P** 202267-54-7P
202267-55-8P 202267-56-9P 202267-57-0P 202267-58-1P
202267-59-2P 202267-61-6P 202267-62-7P 202267-63-8P
202267-64-9P 202267-65-0P 202267-66-1P 202267-67-2P
202267-68-3P 202267-69-4P 202267-70-7P 202267-71-8P
202267-72-9P 202267-73-0P 202267-74-1P 202267-75-2P
202267-76-3P 202267-77-4P 202267-78-5P 202267-79-6P
202267-80-9P 202267-81-0P 202267-82-1P **202267-83-2P**
202267-84-3P 475290-51-8P 475290-52-9P 475290-53-0P
475290-54-1P 475290-55-2P 475290-56-3P
(preparation of adenosine analogs for the treatment of insulin resistance syndrome and diabetes)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

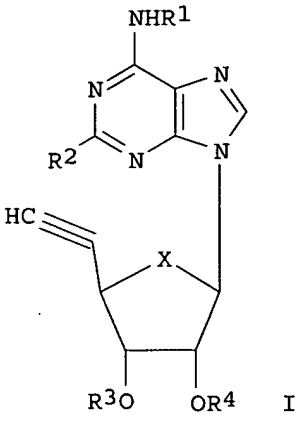
L22 ANSWER 5 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:736264 HCAPLUS
DOCUMENT NUMBER: 137:232864
TITLE: Preparation of nucleosides as human adenosine A1 and A3 receptor agonists
INVENTOR(S): Hall, Adrian; Jandu, Karamjit Singh; Lunnis, Christopher James; Vinader, Maria Victoria; West, Robert Ian
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2002074780	A1	20020926	WO 2002-GB1317	2002 0319
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2441202	AA	20020926	CA 2002-2441202	2002 0319
EP 1370568	A1	20031217	EP 2002-714332	2002 0319
EP 1370568	B1	20051012		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002008169	A	20040302	BR 2002-8169	2002 0319
CN 1501941	A	20040602	CN 2002-806775	2002 0319
NZ 527854	A	20040924	NZ 2002-527854	2002 0319
JP 2004534002	T2	20041111	JP 2002-573789	2002 0319
AT 306492	E	20051015	AT 2002-714332	2002 0319
ZA 2003006769	A	20040618	ZA 2003-6769	2003 0829
NO 2003004182	A	20030919	NO 2003-4182	2003 0919
US 2004162422	A1	20040819	US 2004-471681	2004 0304
PRIORITY APPLN. INFO.:			GB 2001-6871 A	2001 0320
			GB 2001-6875 A	2001 0320
			GB 2001-6877 A	2001 0320

WO 2002-GB1317 W
2002
0319

OTHER SOURCE(S): MARPAT 137:232864
GI



I

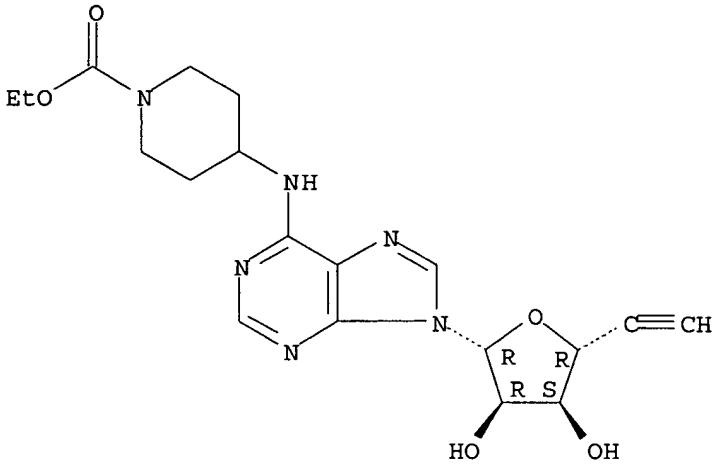
AB Nucleosides I, wherein X represents O or CH2; R1 represents substituted cycloalkyl, cycloalkenyl, Ph, heterocyclic, alkyl, fused bicyclic ring; R2 represents alkyl, halogen, H, alkoxy; R3 and R4 are independently H, alkyl, which are adenosine A1 and A3 receptor agonists, and to their use in therapy. Thus, (2R,3R,4S,5R)-2-[6-[(4-chloro-2-fluorophenyl)amino]-9H-purin-9-yl]-5-ethynyltetrahydrofuran-3,4-diol was prepared as human adenosine A1 and A3 receptor agonist. Title nucleosides were prepared for the treatment of a patient suffering from or susceptible to ischemic heart disease, peripheral vascular disease or stroke or which subject is suffering pain, a CNS disorder.

IT **458566-28-4P**
(preparation of nucleosides as human adenosine A1 and A3 receptor agonists)

RN 458566-28-4 HCAPLUS

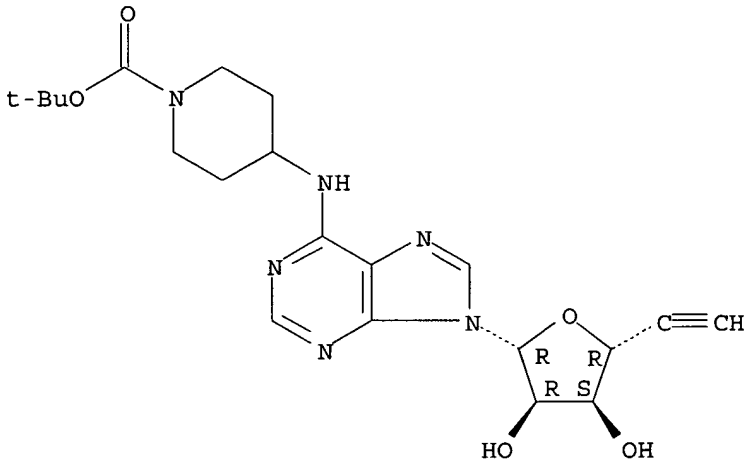
CN 1-Piperidinecarboxylic acid, 4-[[9-(5,6-dideoxy-β-D-ribo-hex-5-ynofuranosyl)-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



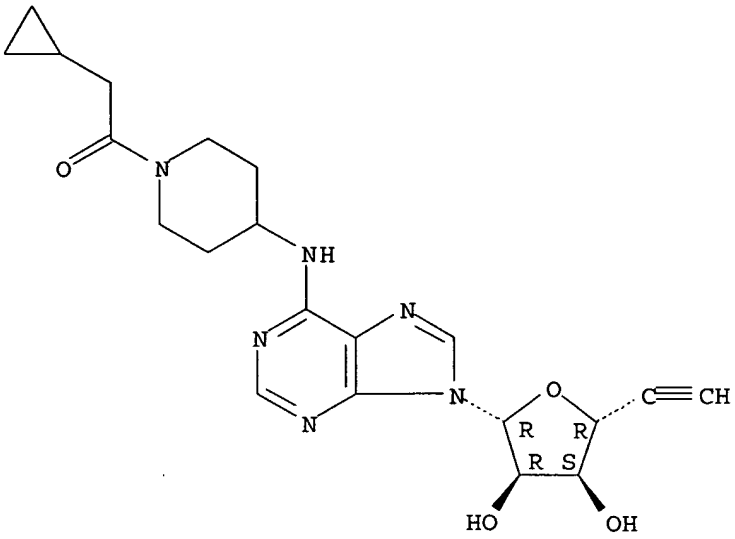
IT **458566-48-8P 458566-49-9P**
(preparation of nucleosides as human adenosine A1 and A3 receptor agonists)
RN 458566-48-8 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-(5,6-dideoxy-β-D-ribo-hex-5-ynofuranosyl)-9H-purin-6-yl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 458566-49-9 HCAPLUS
CN 4-Piperidinamine, 1-(cyclopropylacetyl)-N-[9-(5,6-dideoxy-β-D-ribo-hex-5-ynofuranosyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-16
ICS C07D473-18; C07D473-34; A61K031-70; A61P009-10; A61P025-00
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT 458566-27-3P **458566-28-4P** 458566-29-5P 458566-30-8P
458566-31-9P 458566-32-0P 458566-33-1P 458566-34-2P
458566-35-3P 458566-36-4P 458566-37-5P 458566-38-6P
458566-39-7P 458566-41-1P 458566-42-2P 458566-43-3P
458566-44-4P 458566-45-5P 458566-58-0P 458566-61-5P
458566-62-6P 458566-63-7P 458566-64-8P 458566-65-9P
458566-66-0P 458566-67-1P 458566-68-2P 459409-39-3P
459409-40-6P
(preparation of nucleosides as human adenosine A1 and A3 receptor agonists)
IT 458566-46-6P 458566-47-7P **458566-48-8P**
458566-49-9P 458566-50-2P 458566-51-3P 458566-52-4P
458566-53-5P 458566-54-6P 458566-55-7P 458566-56-8P
458566-57-9P 458566-59-1P 458566-60-4P 458566-69-3P
458566-70-6P 458566-71-7P 458566-72-8P 458566-73-9P
(preparation of nucleosides as human adenosine A1 and A3 receptor agonists)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

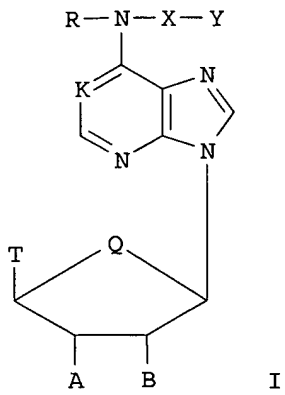
L22 ANSWER 6 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:556109 HCAPLUS
DOCUMENT NUMBER: 137:109451
TITLE: Preparation of adenosine analogs having antihypertensive, cardioprotective, anti-ischemic, and antilipolytic properties
INVENTOR(S): Myers, Michael R.; Maguire, Martin P.; Spada, Alfred P.; Ewing, William R.; Pauls, Henry W.; Choi-Sledeski, Yong Mi
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp., Cont.-in-part of Appl. No. PCT/US97/11320.
CODEN: USXXCO

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099030	A1	20020725	US 2002-104133	20020322
US 6559313	B2	20030506		
WO 9801426	A1	19980115	WO 1997-US11320	19970701
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CZ 292404	B6	20030917	CZ 2001-4373	20011205

PRIORITY APPLN. INFO.:			US 1996-21366P	P 19960708
			WO 1997-US11320	A2 19970701
			CZ 1999-24	A3 19970701

OTHER SOURCE(S): MARPAT 137:109451
GI



I

AB Adenosine derivs. and analogs I (K = N, NO, CH; Q = CH2, O; R = H,

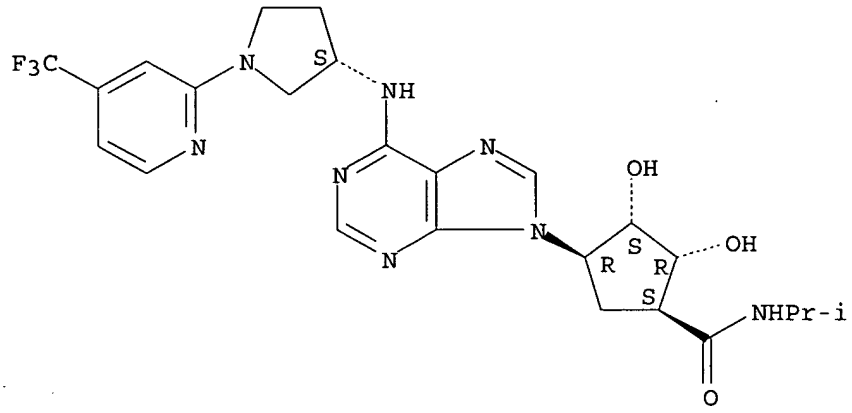
alkyl, allyl, 2-methylallyl, 2-butenyl, cycloalkyl; X = N-containing heterocycle; Y = H, alkyl, aralkyl, aryl, heterocycle, heterocycloalkyl; T = H, alkyl, acyl, thioacyl, halo, carboxyl, alkoxymethyl; A, B = independently H, alkyl, hydroxyalkyl, OH) were prepared as anti-hypertensive, cardioprotective, anti-ischemic, and antilipolytic agents, and for treating hyperlipidemia and hypercholesterolemia. Thus, (2R,3R,4S,5R)-2-hydroxymethyl-5[6-[(1-5-chloropyridin-2-yl)-pyrrolidin-3(S)-ylamino]-purin-9-yl]-tetrahydrofuran-3,4-diol was prepared and tested for its biol. activity (no data).

IT **202267-01-4P 202267-46-7P 202267-53-6P**
202267-83-2P 202267-84-3P
(preparation of adenosine nucleosides as antihypertensives, cardioprotectives, anti-ischemics and anti-lipolytics)

RN 202267-01-4 HCAPLUS

CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-(1-methylethyl)-4-[6-[[(3S)-1-[4-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

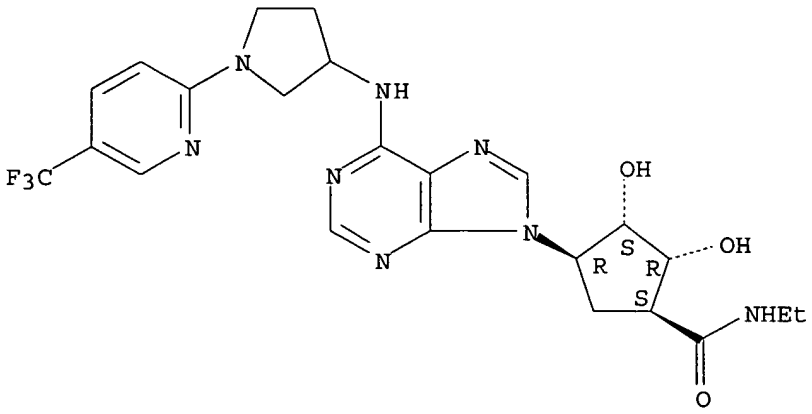
Absolute stereochemistry.



RN 202267-46-7 HCAPLUS

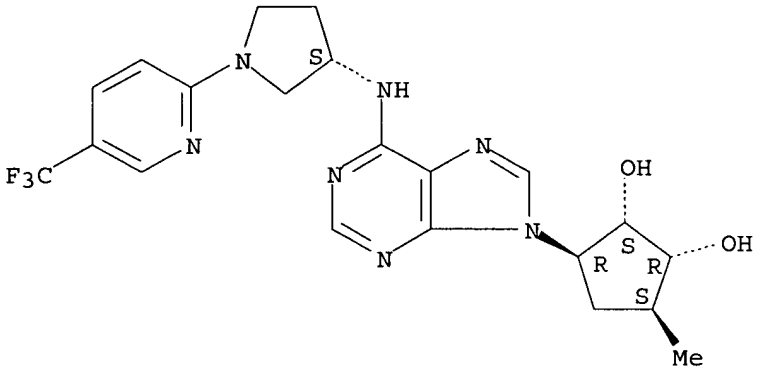
CN Cyclopentanecarboxamide, N-ethyl-2,3-dihydroxy-4-[6-[[1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



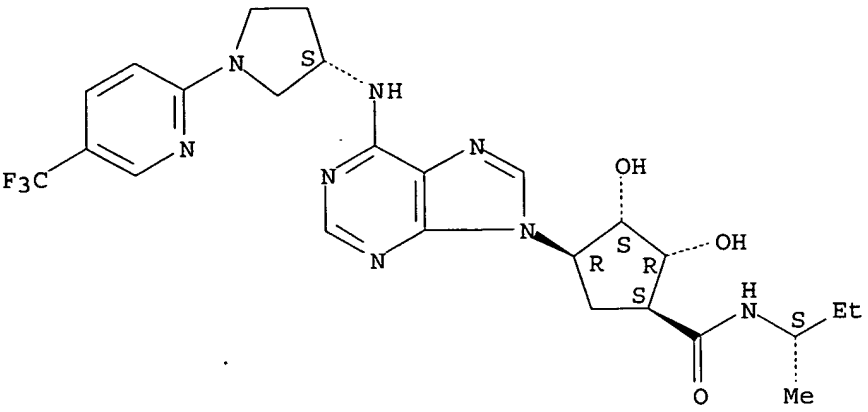
RN 202267-53-6 HCAPLUS
CN 1,2-Cyclopentanediol, 3-methyl-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



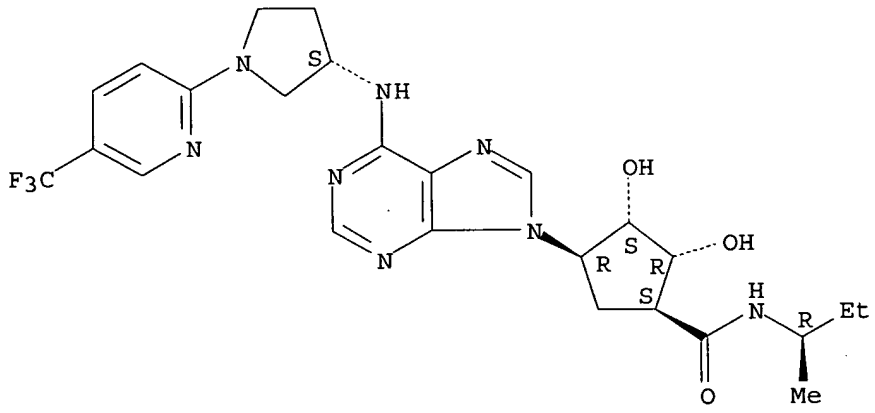
RN 202267-83-2 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1S)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 202267-84-3 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1R)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-7076
ICS A61K031-52; A61K031-4745; C07H019-16; C07D473-34
INCL 514046000; X51-421.021; X51-426.323; X51-426.32; X51-426.322; X54-427.7; X53-6 2.73; X51-430.3; X54-611.8
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT **202267-01-4P** 202267-06-9P 202267-14-9P 202267-16-1P
202267-20-7P 202267-24-1P 202267-30-9P 202267-31-0P
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202267-68-3P 202267-69-4P 202267-70-7P 202267-71-8P
202267-72-9P 202267-73-0P 202267-74-1P 202267-75-2P
202267-76-3P 202267-77-4P 202267-78-5P 202267-79-6P
202267-80-9P 202267-81-0P 202267-82-1P **202267-83-2P**
202267-84-3P
(preparation of adenosine nucleosides as antihypertensives, cardioprotectives, anti-ischemics and anti-lipolytics)

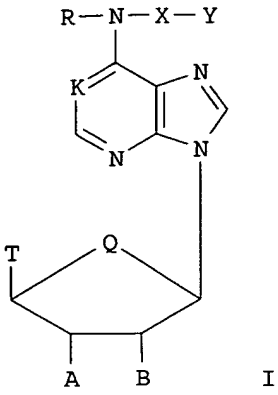
L22 ANSWER 7 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:277985 HCAPLUS
DOCUMENT NUMBER: 132:293976
TITLE: Preparation of adenosine analogues having antihypertensive, cardioprotective, anti-ischemic, and antilipolytic properties
INVENTOR(S): Myers, Michael R.; Maguire, Martin P.; Spada, Alfred P.; Ewing, William R.; Pauls, Heinz W.; Choi-Sledeski, Yong Mi
PATENT ASSIGNEE(S): Aventis Pharmaceuticals Products Inc., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000023447	A1	20000427	WO 1999-US22932	1999 1012
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6376472	B1	20020423	US 1998-174191	1998 1016
AU 9964107	A1	20000508	AU 1999-64107	1999 1012

PRIORITY APPLN. INFO.:		
US 1998-174191	A	1998 1016
US 1996-21366P	P	1996 0708
WO 1997-US11320	A2	1997 0701

WO 1999-US22932 W
1999
1012

OTHER SOURCE(S): MARPAT 132:293976
GI



I

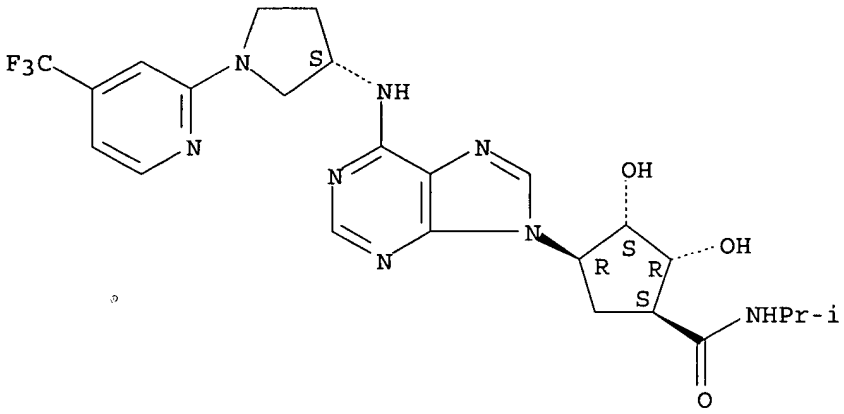
AB Adenosine derivs. and analogs I (K = N, NO, CH; Q = CH2, O; R = H, alkyl, allyl, 2-methylallyl, 2-butenyl, cycloalkyl; X = N-containing heterocycle; Y = H, alkyl, aralkyl, aryl, heterocycle, heterocycloalkyl; T = H, alkyl, acyl, thioacyl, halo, carboxyl, alkoxymethyl; A, B = independently H, alkyl, hydroxyalkyl, OH) were prepared as anti-hypertensive, cardioprotective, anti-ischemic, and antilipolytic agents, and for treating hyperlipidemia and hypercholesterolemia. Thus, (2R,3R,4S,5R)-2-hydroxymethyl-5[6-[(1-5-chloropyridin-2-yl)-pyrrolidin-3(S)-ylamino]-purin-9-yl]-tetrahydrofuran-3,4-diol was prepared and tested for its biol. activity (no data).

IT **202267-01-4P 202267-46-7P 202267-53-6P**
202267-83-2P 202267-84-3P
(preparation of adenosine nucleosides as antihypertensives, cardioprotectives, anti-ischemics and anti-lipolytics)

RN 202267-01-4 HCAPLUS

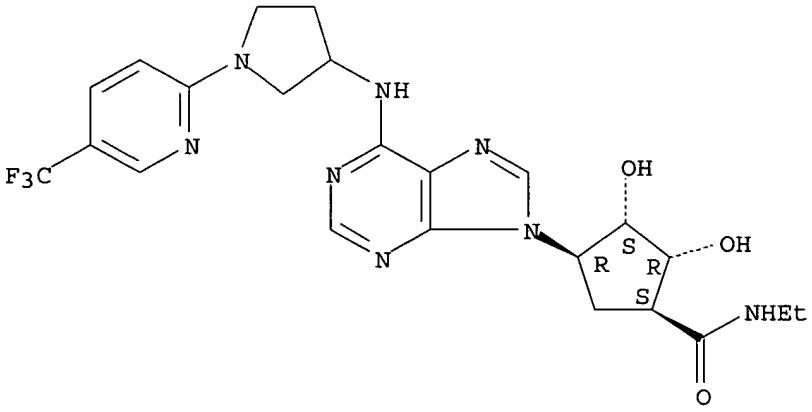
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-(1-methylethyl)-4-[6-[[(3S)-1-[4-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



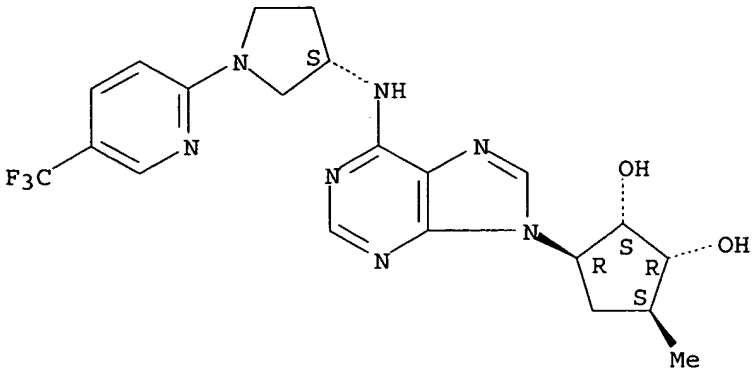
RN 202267-46-7 HCAPLUS
CN Cyclopentanecarboxamide, N-ethyl-2,3-dihydroxy-4-[6-[[1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



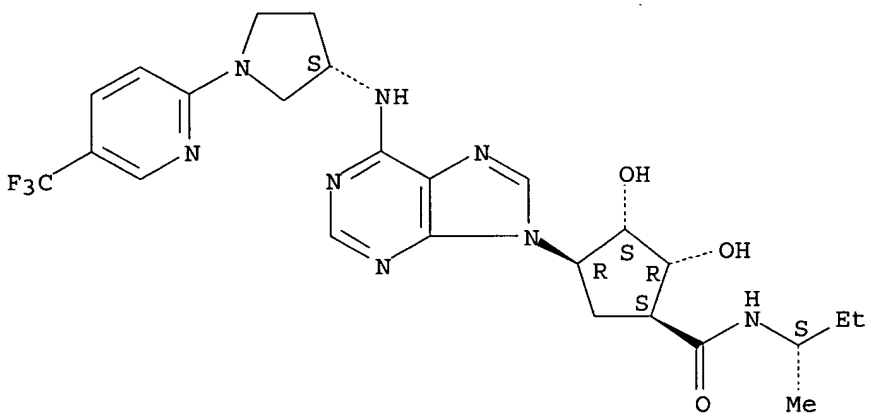
RN 202267-53-6 HCAPLUS
CN 1,2-Cyclopentanediol, 3-methyl-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



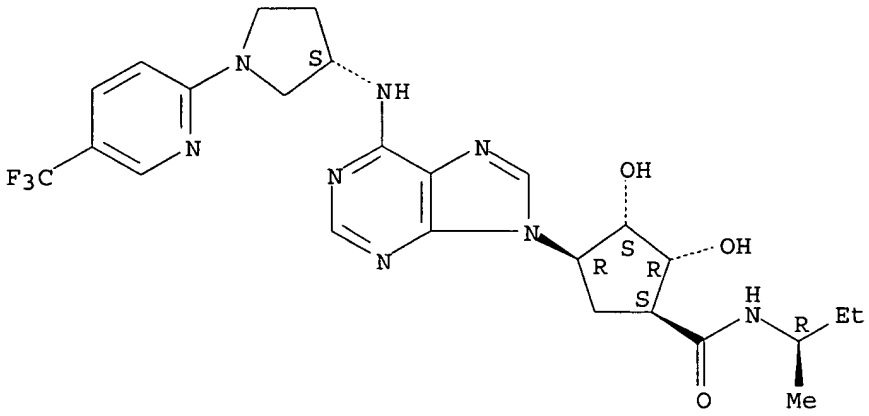
RN 202267-83-2 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1S)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 202267-84-3 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1R)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07D473-34
ICS C07H019-167; A61K031-70; A61K031-52
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT **202267-01-4P** 202267-06-9P 202267-14-9P 202267-16-1P
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202267-32-1P 202267-33-2P 202267-34-3P 202267-35-4P
202267-36-5P 202267-37-6P 202267-38-7P 202267-39-8P
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202267-76-3P 202267-77-4P 202267-78-5P 202267-79-6P
202267-80-9P 202267-81-0P 202267-82-1P **202267-83-2P**
202267-84-3P
(preparation of adenosine nucleosides as antihypertensives, cardioprotectives, anti-ischemics and anti-lipolytics)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 8 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:819388 HCAPLUS
DOCUMENT NUMBER: 132:64480
TITLE: Preparation of adenosine derivatives as antiinflammatory agents
INVENTOR(S): Bays, David Edmund; Cousins, Richard Peter Charles; Dyke, Hazel Joan; Eldred, Colin David; Judkins, Brian David; Pass, Martin; Pennell, Andrew Michael Kenneth
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: PCT Int. Appl., 161 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9967262	A1	19991229	WO 1999-EP4182	1999 0621
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2335520	AA	19991229	CA 1999-2335520	1999 0621
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AU 758018	B2	20030313		
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EP 1090019	A1	20010411	EP 1999-927999	1999 0621
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TR 200100449	T2	20010821	TR 2001-200100449	1999 0621
EE 200000784	A	20020415	EE 2000-784	1999 0621
JP 2002518509	T2	20020625	JP 2000-555913	1999 0621
JP 3378240	B2	20030217		
JP 2003040891	A2	20030213	JP 2002-170486	1999 0621
NZ 508915	A	20030926	NZ 1999-508915	1999 0621
EP 1447407	A1	20040818	EP 2004-76465	1999 0621
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PT 1090019	T	20050131	PT 1999-927999	1999 0621
ES 2226399	T3	20050316	ES 1999-927999	

				1999 0621
CN 1616459	A	20050518	CN 2004-10011939	1999 0621
TW 541312	B	20030711	TW 1999-88111178	1999 0701
ZA 2000007514	A	20020123	ZA 2000-7514	2000 1214
NO 2000006520	A	20010214	NO 2000-6520	2000 1220
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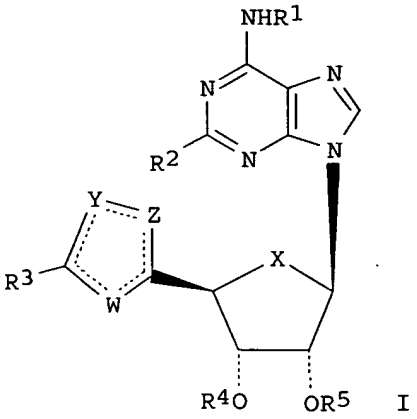
HR 20000896	B1	20060331		
BG 105155	A	20010928	BG 2001-105155	2001 0115
US 6492348	B1	20021210	US 2001-736018	2001 0306
HK 1034978	A1	20050408	HK 2001-105686	2001 0814
US 2003096788	A1	20030522	US 2002-217107	2002 0813
US 6677316	B2	20040113		
PRIORITY APPLN. INFO.:			GB 1998-13554 A	1998 0623
			EP 1999-927999 A3	1999 0621
			JP 2000-555913 A3	1999 0621
			WO 1999-EP4182 W	1999 0621
			US 2001-736018 A1	2001 0306

OTHER SOURCE(S): MARPAT 132:64480
GI



I

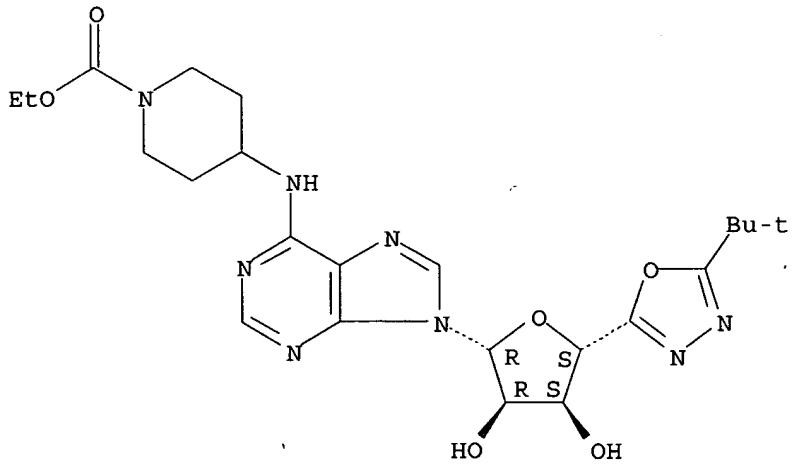
AB Adenosine derivs. I (X = O, CH2; Y and Z = O, N, CH, alkylamine; W = heteroatom; R1 = H, alkylcycloalkyl, heterocycle, fused bicyclic, substituted phenyl) which is an agonist at the adenosine A1 and A3 receptors. Thus, (2S,3S,4R,5R)-2-(5-tert-butyl-[1,3,4]oxadiazol-2-yl)-5[6-(tetrahydropyran-4-ylamino)-purin-9-yl]tetrahydrofuran-3,4-diol was prepared as adenosine A1 and A3 receptors (ECR are resp. 4.16 and 152).

IT **253124-34-4P 253124-44-6P 253124-59-3P**
253124-70-8P 253124-92-4P 253124-95-7P
253125-11-0P 253125-15-4P 253125-22-3P
253125-26-7P 253125-29-0P 253125-60-9P
253125-78-9P 253125-88-1P 253125-96-1P
253125-97-2P 253125-98-3P 253126-00-0P
253126-15-7P 253126-18-0P 253126-19-1P
253126-20-4P 253126-21-5P
(preparation of adenosine derivs. as antiinflammatory agents)

RN 253124-34-4 HCAPLUS

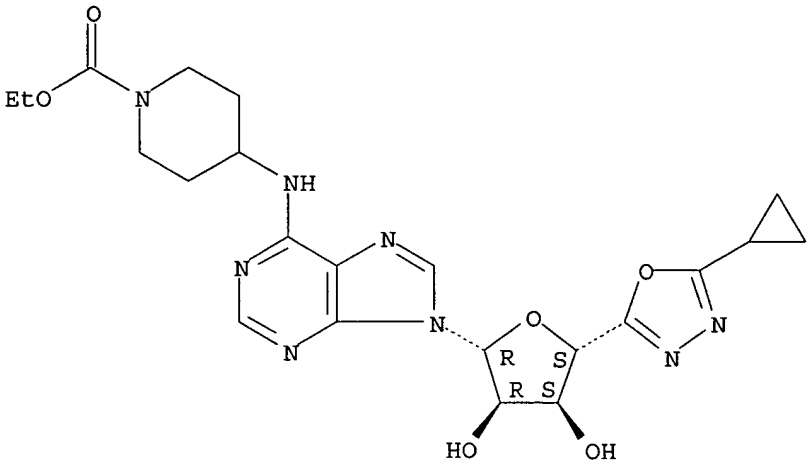
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-[5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2-yl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



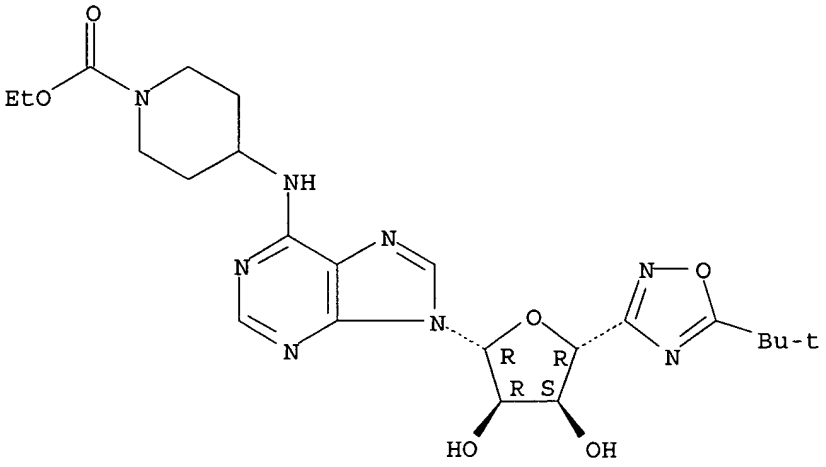
RN 253124-44-6 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-(5-cyclopropyl-1,3,4-oxadiazol-2-yl)tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



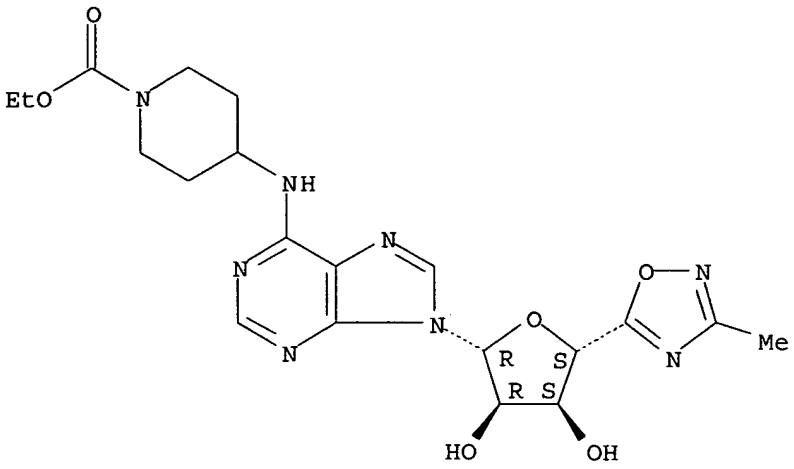
RN 253124-59-3 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5R)-5-[5-(1,1-dimethylethyl)-1,2,4-oxadiazol-3-yl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



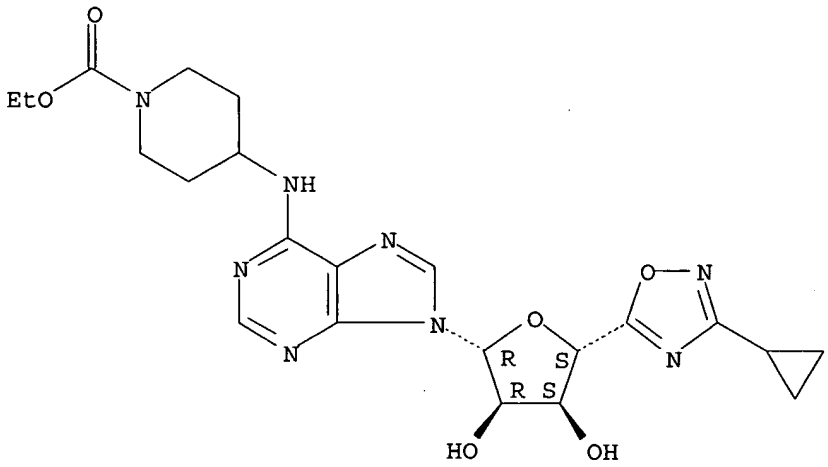
RN 253124-70-8 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-tetrahydro-3,4-dihydroxy-5-(3-methyl-1,2,4-oxadiazol-5-yl)-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



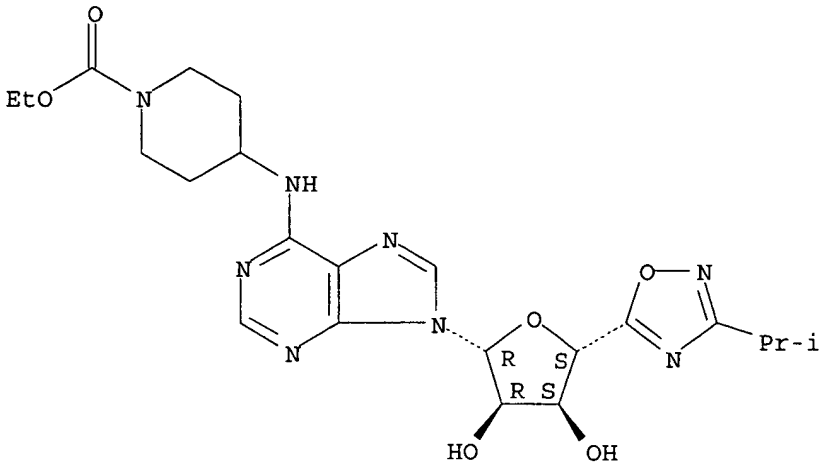
RN 253124-92-4 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-(3-cyclopropyl-1,2,4-oxadiazol-5-yl)tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



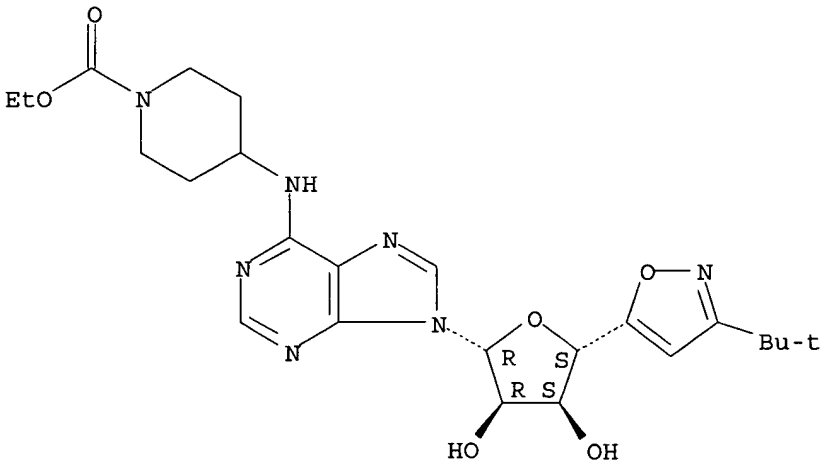
RN 253124-95-7 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-tetrahydro-3,4-dihydroxy-5-[3-(1-methylethyl)-1,2,4-oxadiazol-5-yl]-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



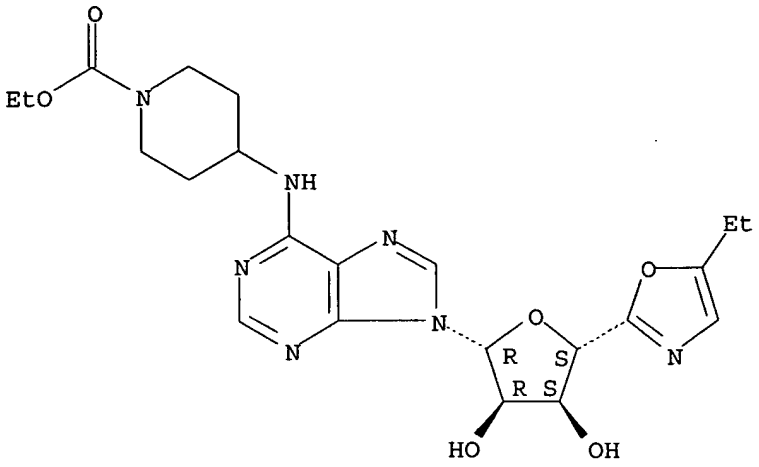
RN 253125-11-0 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



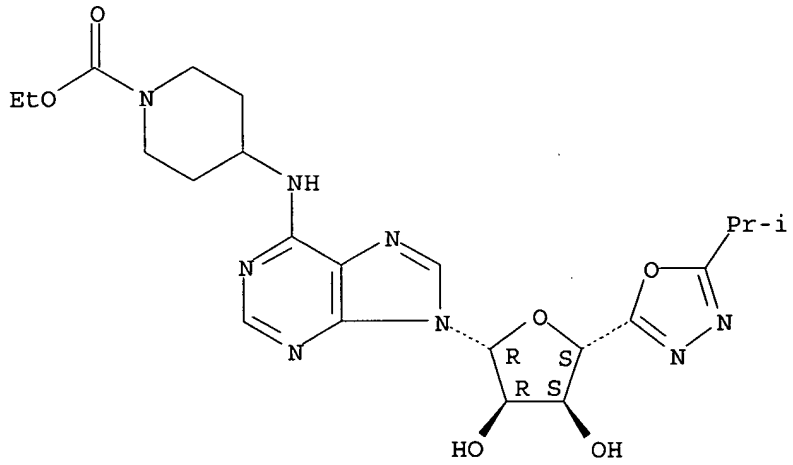
RN 253125-15-4 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-(5-ethyl-2-oxazolyl)tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



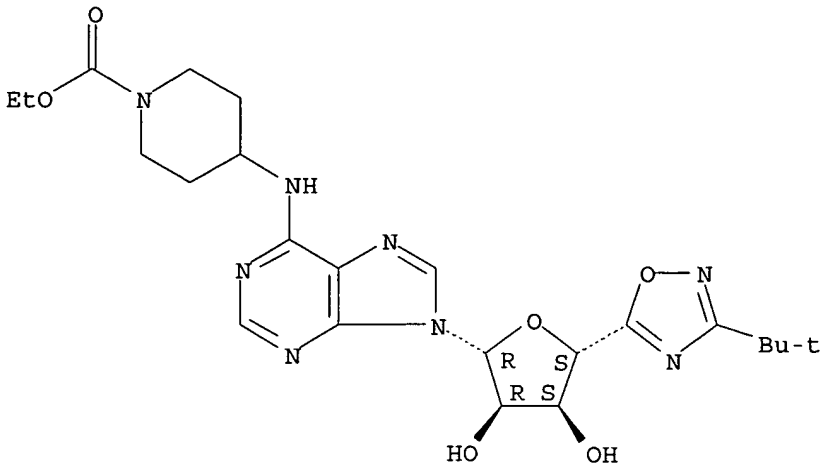
RN 253125-22-3 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-tetrahydro-3,4-dihydroxy-5-[5-(1-methylethyl)-1,3,4-oxadiazol-2-yl]-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



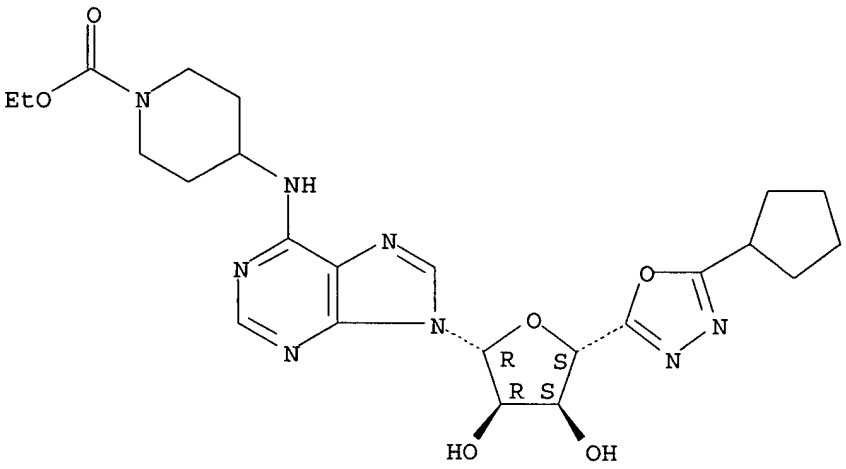
RN 253125-26-7 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-1,2,4-oxadiazol-5-yl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



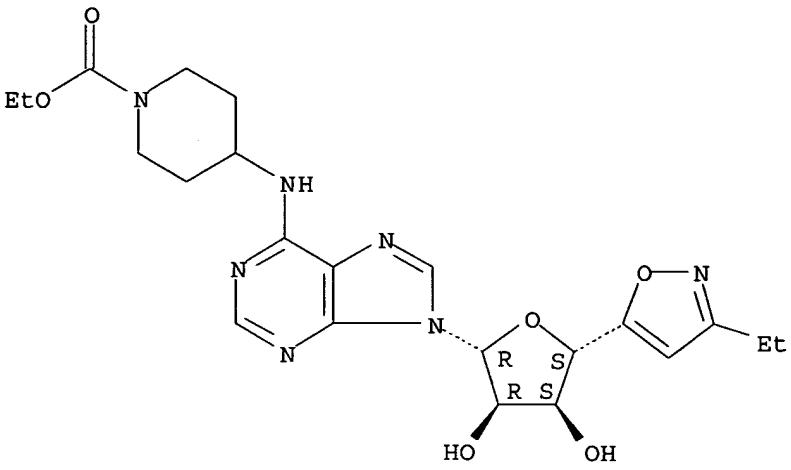
RN 253125-29-0 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-(5-cyclopentyl-1,3,4-oxadiazol-2-yl)tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



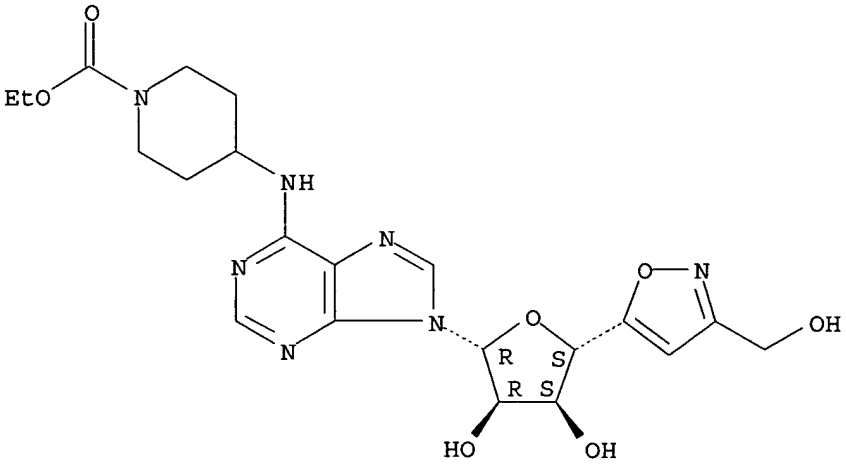
RN 253125-60-9 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-(3-ethyl-5-isoxazolyl)tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



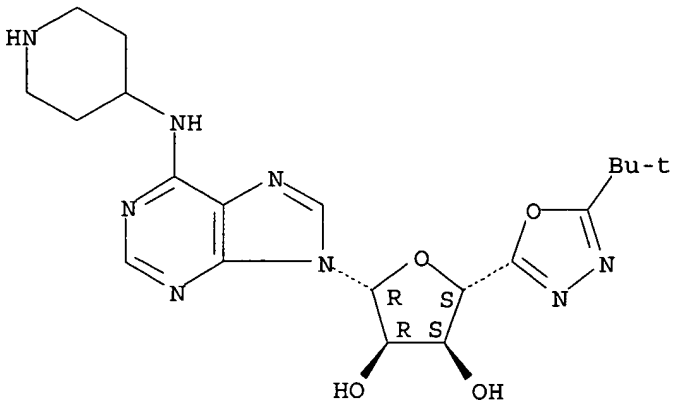
RN 253125-78-9 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-tetrahydro-3,4-dihydroxy-5-[3-(hydroxymethyl)-5-isoxazolyl]-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



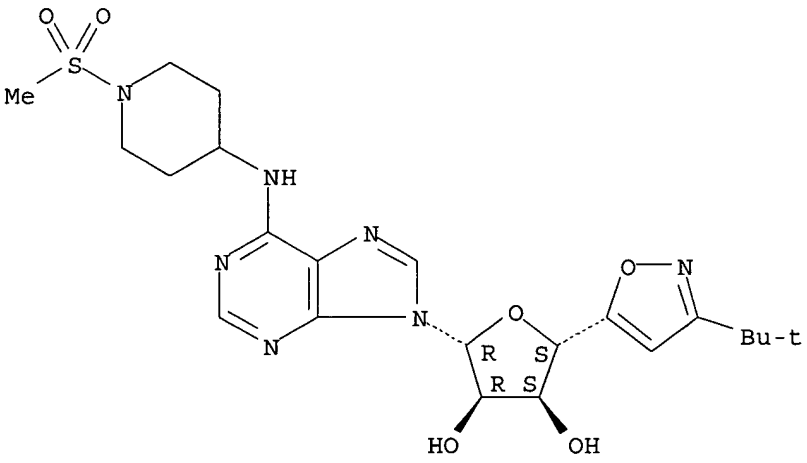
RN 253125-88-1 HCAPLUS
CN 3,4-Furandiol, 2-[5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2-yl]tetrahydro-5-[6-(4-piperidinylamino)-9H-purin-9-yl]-, (2S,3S,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



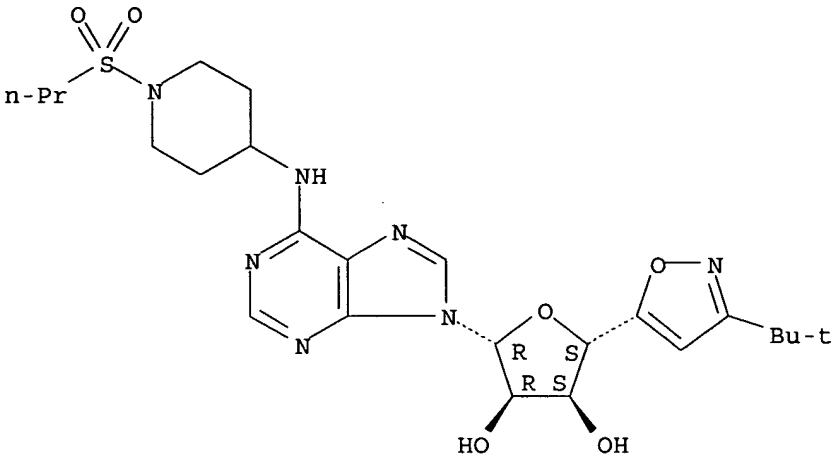
RN 253125-96-1 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]-1-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



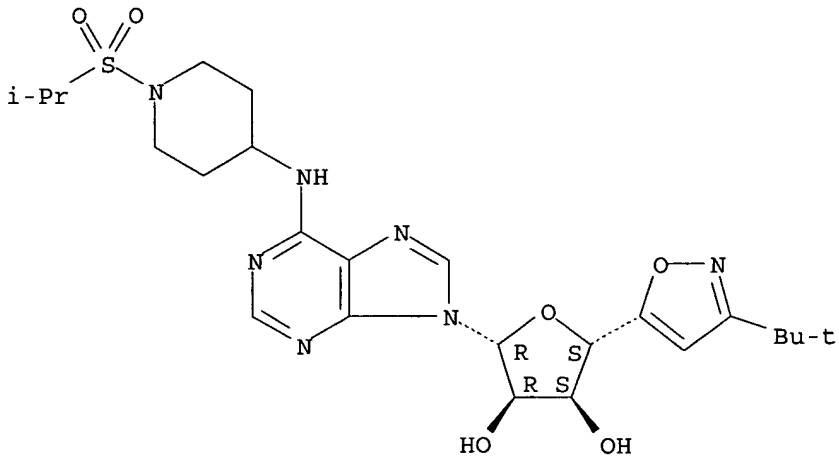
RN 253125-97-2 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]-1-(propylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



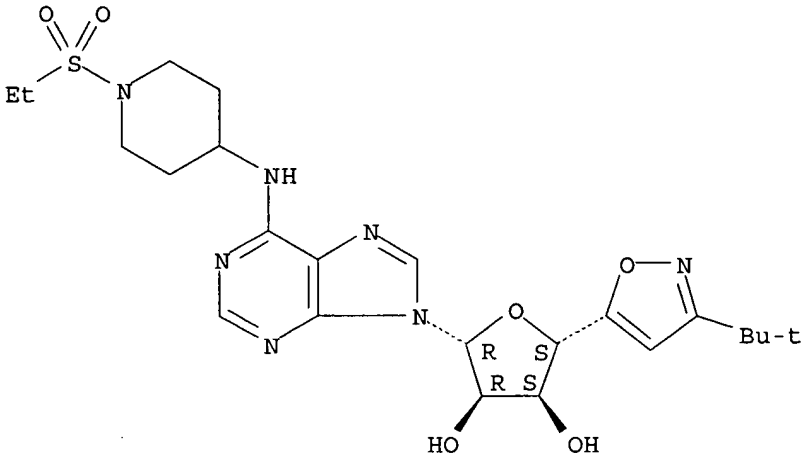
RN 253125-98-3 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]-1-[(1-methylethyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



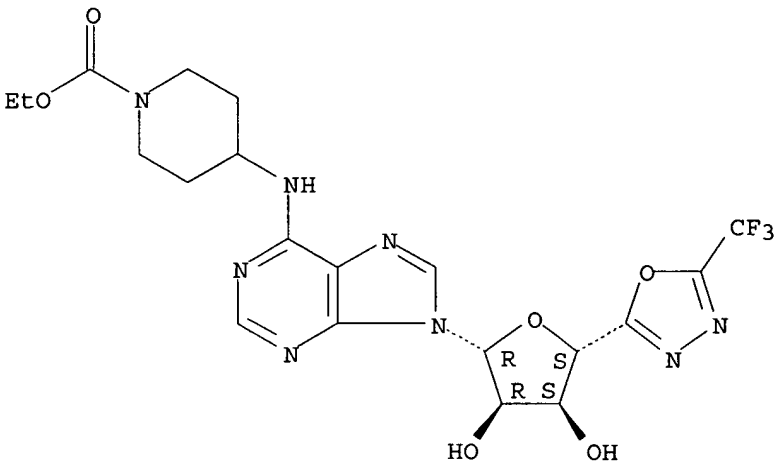
RN 253126-00-0 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]-1-(ethylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



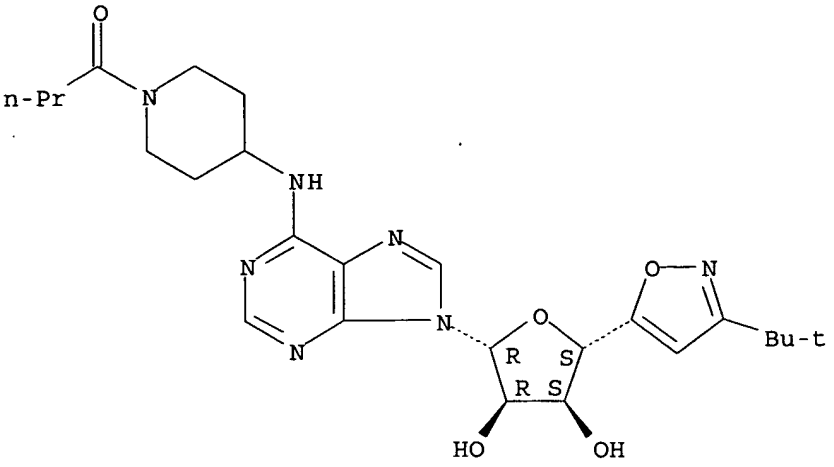
RN 253126-15-7 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-tetrahydro-3,4-dihydroxy-5-[5-(trifluoromethyl)-1,3,4-oxadiazol-2-yl]-2-furanyl]-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



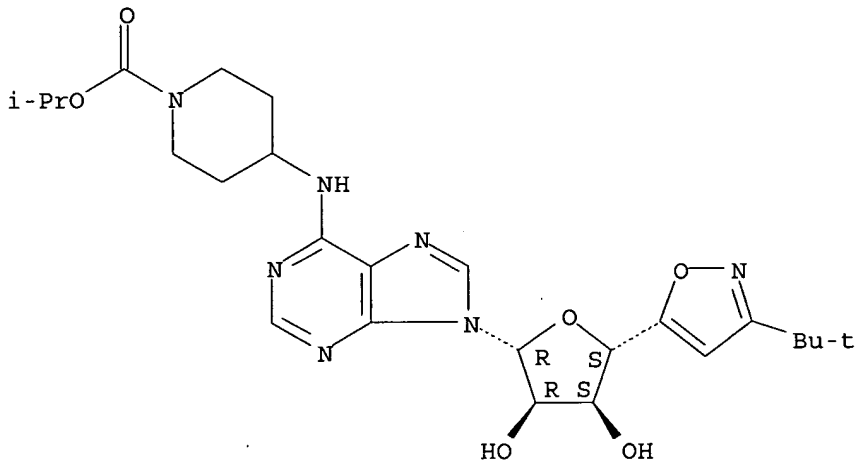
RN 253126-18-0 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]-1-(1-oxobutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



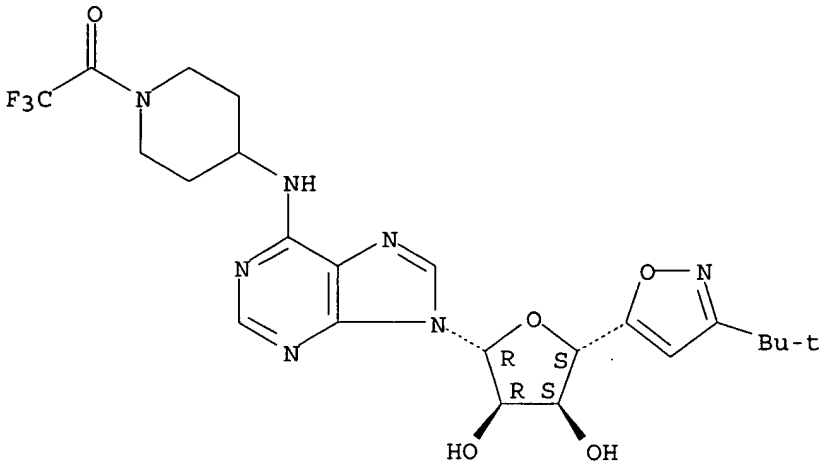
RN 253126-19-1 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



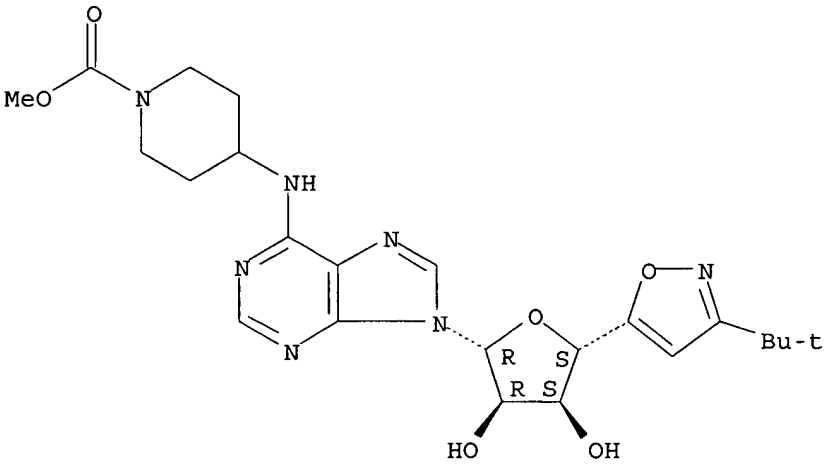
RN 253126-20-4 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]-1-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



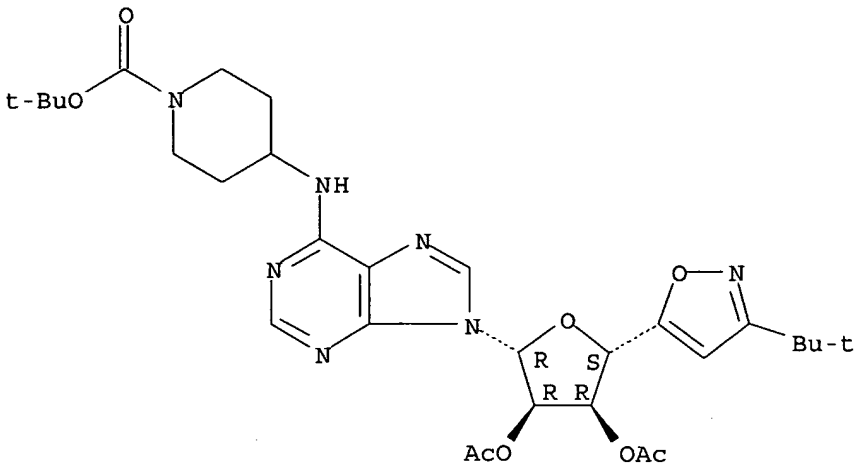
RN 253126-21-5 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4S,5S)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-3,4-dihydroxy-2-furanyl]-9H-purin-6-yl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



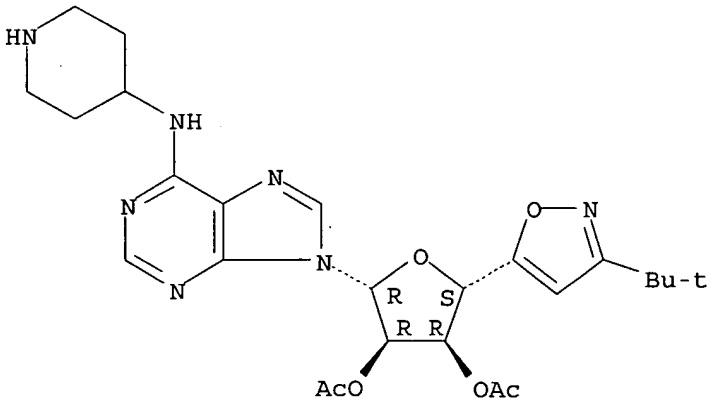
IT **253127-12-7 253127-13-8 253127-14-9**
(preparation of adenosine derivs. as antiinflammatory agents)
RN 253127-12-7 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[9-[(2R,3R,4R,5S)-3,4-bis(acetyloxy)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-2-furanyl]-9H-purin-6-yl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



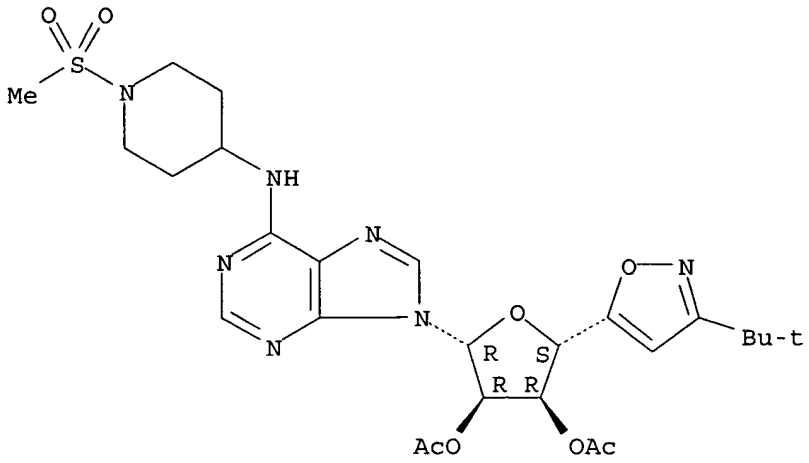
RN 253127-13-8 HCAPLUS
CN 3,4-Furandiol, 2-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-5-[6-(4-piperidinylamino)-9H-purin-9-yl]-, diacetate (ester), (2S,3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 253127-14-9 HCAPLUS
CN 4-Piperidinamine, N-[9-[(2R,3R,4R,5S)-3,4-bis(acetyloxy)-5-[3-(1,1-dimethylethyl)-5-isoxazolyl]tetrahydro-2-furanyl]-9H-purin-6-yl]-1-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-16
ICS A61K031-70

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63

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(preparation of adenosine derivs. as antiinflammatory agents)

IT 75-64-9, tert-Butylamine, reactions 78-81-9, Isobutylamine 78-96-6, 1-Amino-2-propanol 87-42-3, 6-Chloropurine 107-29-9, Acetaldoxime 108-03-2, 1-Nitropropane 108-24-7, Acetic anhydride 110-71-4, DME 123-38-6, Propionaldehyde, reactions 124-63-0, Methanesulfonyl chloride 367-25-9, 2,4-Difluoroaniline 616-24-0, 1-Ethylpropylamine 917-92-0, 3,3-Dimethyl-1-butyne 2592-95-2, 1-Hydroxybenzotriazole 3056-18-6 3182-95-4, (S)-Phenylalaninol 5451-40-1, 2,6-Dichloropurine 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 7803-49-8, Hydroxylamine, reactions 7803-57-8, Hydrazine hydrate 13552-21-1, 1-Amino-2-butanol 14169-12-1 16357-59-8 25952-53-8, EDAP 28440-13-3 42826-42-6 42956-75-2, tert-Butylamidoxime 57946-56-2, 4-Chloro-2-fluoro-aniline 68327-04-8 68673-90-5 74213-24-4, Dibromoformaldoxime 75003-90-6 87120-72-7 91893-69-5 97716-24-0 108661-54-7 120355-42-2 253127-10-5 253127-11-6 **253127-12-7** **253127-13-8 253127-14-9** 253127-15-0 253127-16-1 253127-17-2
(preparation of adenosine derivs. as antiinflammatory agents)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:325950 HCAPLUS
DOCUMENT NUMBER: 130:338350
TITLE: Preparation of deoxyfluoro nucleosides as adenosine A1 receptors
INVENTOR(S): Cousins, Richard Peter Charles; Cox, Brian; Eldred, Colin David; Pennell, Andrew Michael Kenneth
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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OTHER SOURCE(S): MARPAT 130:338350
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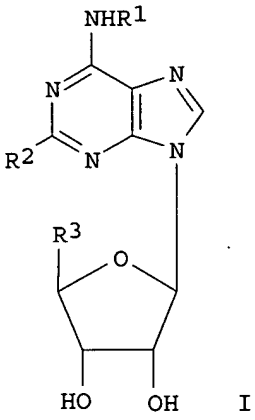


I

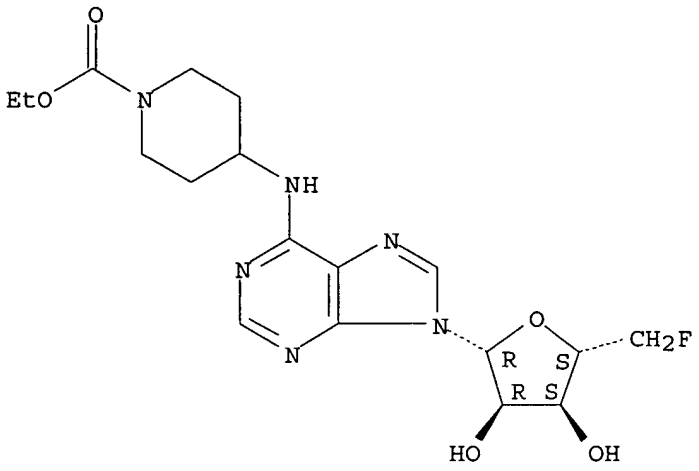
AB Deoxyfluoro nucleosides I which are agonists at the adenosine A1 receptor wherein R1 represents cycloalkyl, heterocylic,alkyl, bicyclic heterocycle, aryl; R2 represents C1-3 alkyl, halogen or hydrogen; R3 represents a fluorinated straight or branched alkyl group of 1-6 carbon atoms and salts and solvates thereof, in particular, physiol. acceptable solvates and salts thereof. These compds. are agonists at the Adenosine A1 receptor. Thus, 5'-deoxy-5'-fluoro-N-(tetrahydro-pyran-4-yl)-adenosine was prepared and tested as adenosine A1 receptor (equipotent concentration ratio relative to NECA = 1.9).

IT **223774-77-4P**
(preparation of deoxyfluoro nucleosides as adenosine A1 receptors)

RN 223774-77-4 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[9-(5-deoxy-5-fluoro-β-D-ribofuranosyl)-9H-purin-6-yl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H019-00
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
IT 223774-67-2P 223774-68-3P 223774-69-4P 223774-70-7P
223774-71-8P 223774-72-9P 223774-74-1P 223774-75-2P
223774-76-3P **223774-77-4P** 223774-78-5P 223774-79-6P
223774-81-0P 223774-82-1P 223774-83-2P 223774-84-3P
223774-85-4P 223774-87-6P 223774-88-7P 223774-89-8P
223774-90-1P 223774-91-2P 223774-92-3P 223774-93-4P
224045-28-7P 224045-30-1P 224045-32-3P
(preparation of deoxyfluoro nucleosides as adenosine A1 receptors)

L22 ANSWER 10 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:65893 HCAPLUS
DOCUMENT NUMBER: 128:140967
TITLE: Preparation of adenosine nucleosides as antihypertensives, cardioprotectives, anti-ischemics and antilipolytics
INVENTOR(S): Myers, Michael R.; Maguire, Martin P.; Spada, Alfred P.; Ewing, William R.; Pauls, Henry W.; Choi-Sledeski, Yong-Mi
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9801426	A1	19980115	WO 1997-US11320	19970701

W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

CA 2259538	AA	19980115	CA 1997-2259538	1997 0701
AU 9736454	A1	19980202	AU 1997-36454	1997 0701
AU 746590	B2	20020502		
EP 912520	A1	19990506	EP 1997-933212	1997 0701
EP 912520	B1	20030507		

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BR 9710156	A	19990810	BR 1997-10156	1997 0701
CN 1228770	A	19990915	CN 1997-197444	1997 0701
JP 2000514801	T2	20001107	JP 1998-505247	1997 0701
AP 903	A	20001124	AP 1998-1426	1997 0701

W: GH, KE, LS, MW, SD, SZ, UG, ZW

CZ 291785	B6	20030514	CZ 1999-24	1997 0701
AT 239725	E	20030515	AT 1997-933212	1997 0701
ES 2199365	T3	20040216	ES 1997-933212	1997 0701
US 6376472	B1	20020423	US 1998-174191	1998 1016
NO 9900063	A	19990308	NO 1999-63	1999 0107
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KR 2000023635	A	20000425	KR 1999-700085	1999 0108
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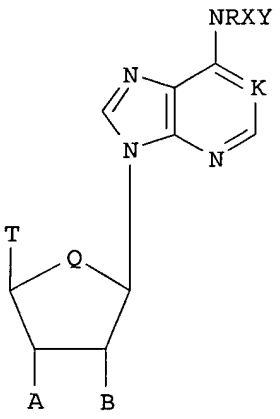
US 2002099030	A1	20020725	US 2002-104133	2002 0322
US 6559313	B2	20030506		
PRIORITY APPLN. INFO.:			US 1996-21366P P	1996

0708

CZ 1999-24 A3
1997
0701

WO 1997-US11320 W
1997
0701

OTHER SOURCE(S): MARPAT 128:140967
GI



I

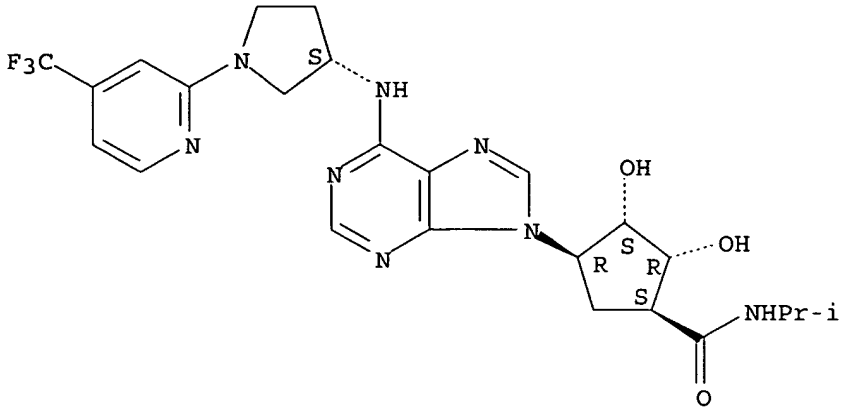
AB Adenosine derivs. and analogs I (K = N, NO, CH; Q = CH2, O; R = H, alkyl, allyl, 2-methyl-allyl, 2-butenyl, cycloalkyl; X = N-containing heterocycle; Y = H, alkyl, aralkyl, aryl, heterocycle, hetero-cycloalkyl; T = H, alkyl, acyl, thioacyl, halo, carboxyl, alkoxymethyl; A, B = independently H, alkyl, hydroxyalkyl, OH) were prepared as anti-hypertensive, cardioprotective, anti-ischemic, and antilipolytic agents, and treating hyperlipidemia and hypercholesterolemia. Thus, (2R,3R,4S,5R)-2-hydroxymethyl-5[6-[(1-5-chloropyridin-2-yl)-pyrrolidin-3(S)-ylamino]-purin-9-yl]-tetrahydrofuran-3,4-diol was prepared and tested for its biol. activity (no data).

IT **202267-01-4P 202267-46-7P 202267-53-6P**
202267-83-2P 202267-84-3P
(preparation of adenosine nucleosides as antihypertensives cardioprotectives antiischemics and antilipolytics)

RN 202267-01-4 HCAPLUS

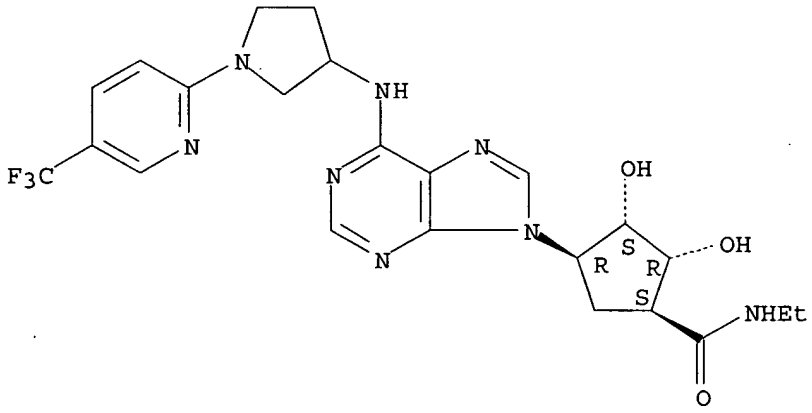
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-(1-methylethyl)-4-[6-[[(3S)-1-[4-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



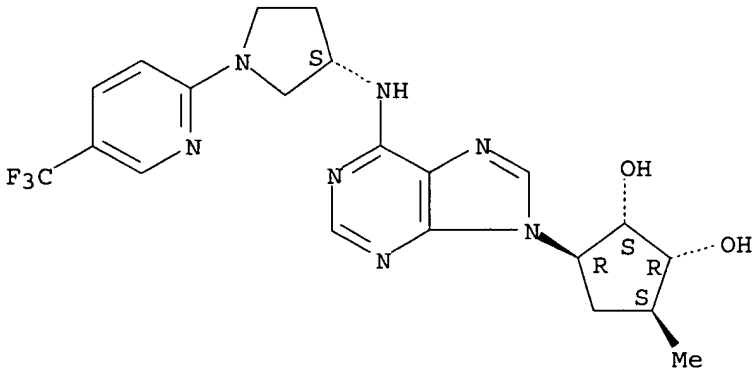
RN 202267-46-7 HCAPLUS
CN Cyclopentanecarboxamide, N-ethyl-2,3-dihydroxy-4-[6-[[1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



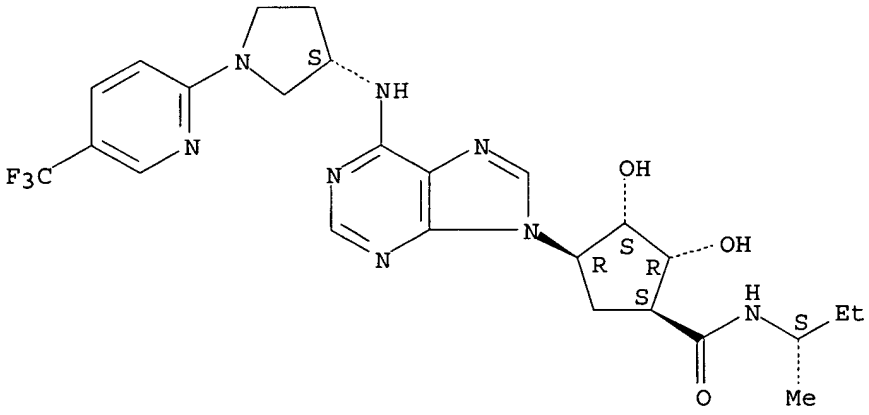
RN 202267-53-6 HCAPLUS
CN 1,2-Cyclopentanediol, 3-methyl-5-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



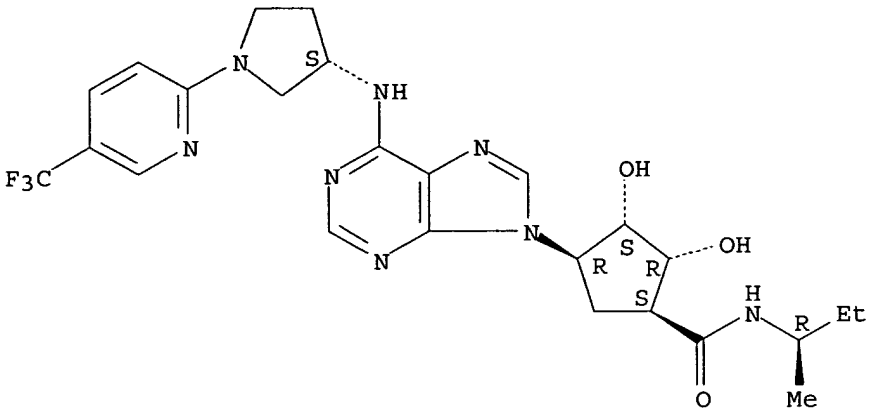
RN 202267-83-2 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1S)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 202267-84-3 HCAPLUS
CN Cyclopentanecarboxamide, 2,3-dihydroxy-N-[(1R)-1-methylpropyl]-4-[6-[[(3S)-1-[5-(trifluoromethyl)-2-pyridinyl]-3-pyrrolidinyl]amino]-9H-purin-9-yl]-, (1S,2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07D227-10
ICS C07D471-04; C07D473-34; A61K031-52
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
IT **202267-01-4P** 202267-06-9P 202267-14-9P 202267-16-1P
202267-20-7P 202267-24-1P 202267-30-9P 202267-31-0P
202267-32-1P 202267-33-2P 202267-34-3P 202267-35-4P
202267-36-5P 202267-37-6P 202267-38-7P 202267-39-8P
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202267-44-5P 202267-45-6P **202267-46-7P** 202267-47-8P
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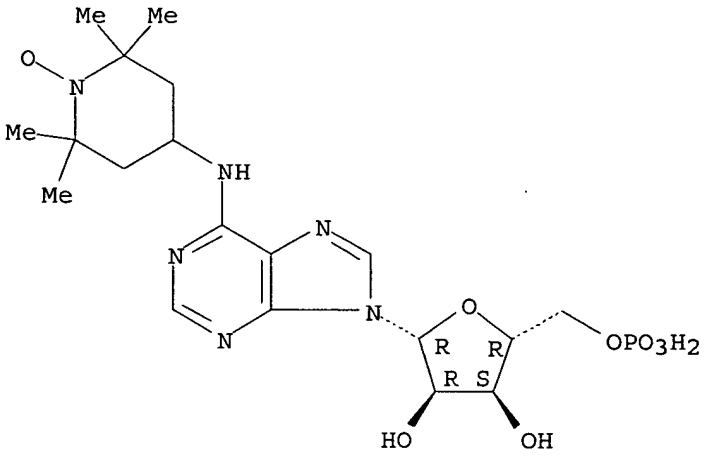
202267-76-3P 202267-77-4P 202267-78-5P 202267-79-6P
202267-80-9P 202267-81-0P 202267-82-1P **202267-83-2P**
202267-84-3P
(preparation of adenosine nucleosides as antihypertensives cardioprotectives antiischemics and antilipolytics)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 11 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:238554 HCAPLUS
DOCUMENT NUMBER: 120:238554
TITLE: Mobility and Orientation of Spin Probes Attached to Nucleotides Incorporated into Actin
AUTHOR(S): Naber, Nariman; Cooke, Roger
CORPORATE SOURCE: Cardiovascular Research Institute, University of California, San Francisco, CA, 94143-0524, USA
SOURCE: Biochemistry (1994), 33(13), 3855-61
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Each actin mol. contains a nucleotide, tightly bound in a deep cleft that divides the mol. To probe conformational changes

within this region of the mol., the authors have incorporated two spin label analogs of ATP into actin. In both analogs the spin label was attached to the 6 position on the adenine ring, either directly (6nSLATP) or via a longer thioacetamido linker (6sSLATP). ESR spectra of randomly oriented actin filaments showed that both the probes possessed considerable rotational mobility relative to the protein surface. The 6nSLADP has two degrees of rotational mobility that can be approx. modeled by rapid diffusion within cones with half angles of 30° and 42°. The 6sSLADP displayed one degree of rotational mobility approximated by rapid motion within a cone with a half-angle of 38°. The rotational mobility of the probes is determined by the protein structure surrounding them, and changes in this structure should alter the mobility. The mobility of the probes was unchanged by addition of 20 mM Pi, which forms an ADP-Pi complex. However, binding of myosin heads (S1) shifted the population of 6nSLADP toward the more highly restricted cone, while binding of DNase-I shifted it toward the less restricted cone. The authors conclude that this region of actin is unchanged by binding of phosphate, while the binding of S1 or DNase-I produces only a modest shift in conformation. When actin filaments were oriented by flow into capillaries, the spectra were strongly dependent on the orientation of the capillary relative to the magnetic field of the spectrometer, showing that although the probes are mobile, the average angles of all the probes are similar, calculated as 70° for the 6nSLADP and 67° for 6sSLADP. These results show that the nucleotide region is highly aligned in the oriented gels.

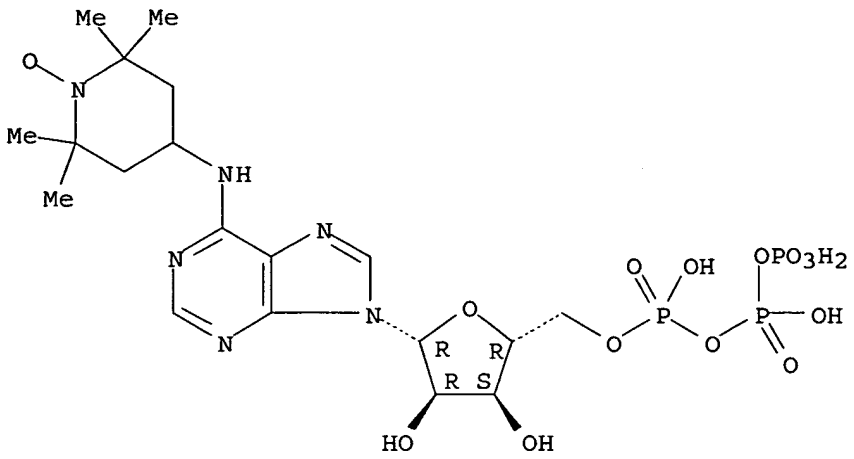
IT **54187-54-1P**
(preparation and conversion to triphosphate)
RN 54187-54-1 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **33913-54-1P**
(preparation and incorporation into actin nucleotide-binding region)
RN 33913-54-1 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 6-3 (General Biochemistry)
IT **54187-54-1P**
(preparation and conversion to triphosphate)
IT **33913-54-1P**
(preparation and incorporation into actin nucleotide-binding region)

L22 ANSWER 12 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:138814 HCAPLUS
DOCUMENT NUMBER: 114:138814
TITLE: Spatial arrangement of coenzyme and substrates bound to L-3-hydroxyacyl-CoA dehydrogenase as studied by spin-labeled analogs of NAD+ and CoA
AUTHOR(S): Hartmann, Dagmar; Philipp, Reinhard; Schmadel, Klaus; Birktoft, J.; Banaszak, Leonard J.; Trommer, Wolfgang E.
CORPORATE SOURCE: Fachbereich Chem., Univ. Kaiserslautern, Kaiserslautern, D-6750, Germany
SOURCE: Biochemistry (1991), 30(11), 2782-90
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of nitroxide spin-labeled derivs. of S-acetoacetyl-CoA, S-acetoacetylpantetheine, and S-acetoacetylcysteamine is described. These compds. are active substrates of L-3-hydroxyacyl-CoA dehydrogenase (EC 1.1.1.35) exhibiting Vmax values form 20% to 70% of S-acetoacetyl-CoA itself. S-Acetoacetylpantetheine and S-acetoacetylcysteamine form binary complexes with the enzyme and exhibit ESR spectra typical for immobilized nitroxides. In the case of spin-labeled pantetheine, the radical is more mobile. When spin-labeled substrates are bound simultaneously to each active site of this dimeric enzyme, spin-spin interactions differentiate between 2 alternate orientations of the substrate. The fatty acid moiety is thought to be located in a cleft between 2 domains whereas a large part of the CoA moiety probably extends into the solution NAD+, spin-labeled at N6 of the adenine ring, is an active coenzyme of L-3-hydroxyacyl-CoA dehydrogenase (60% Vmax). Complexes with the enzyme exhibit ESR spectra typical of highly immobilized nitroxides. Binding of coenzyme NAD+ causes conformational

changes of the binary enzyme/substrate complex as revealed by changes in the ESR spectrum of spin-labeled S-acetoacetylpantetheine.

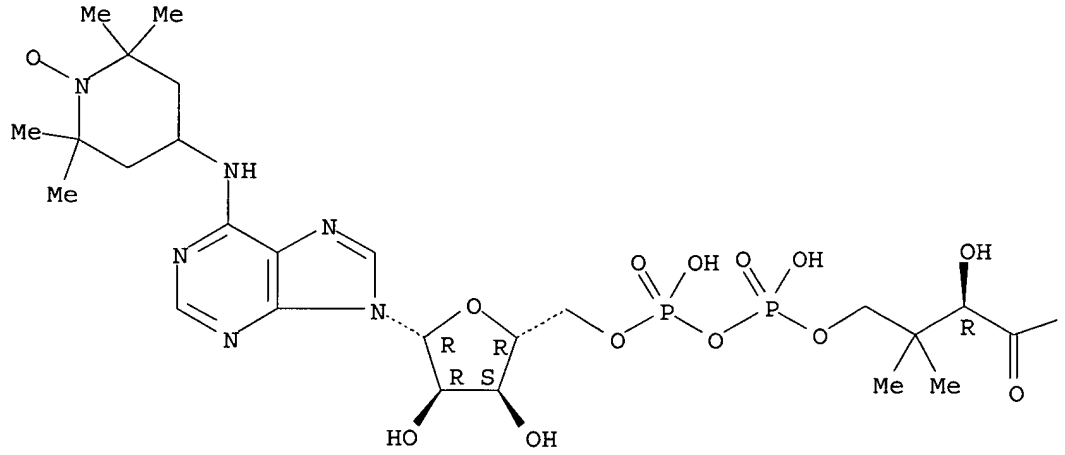
IT **132439-12-4P**
(preparation and hydroxyacyl-CoA-dehydrogenase binding by, coenzyme and substrate spatial arrangement in enzyme active site in relation to)

RN 132439-12-4 HCAPLUS

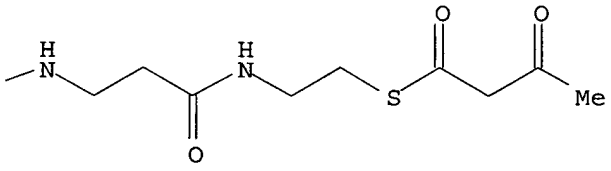
CN Coenzyme A, N-(2,2,6,6-tetramethyl-1-oxy-4-piperidinyl)-, S-(3-oxobutanoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

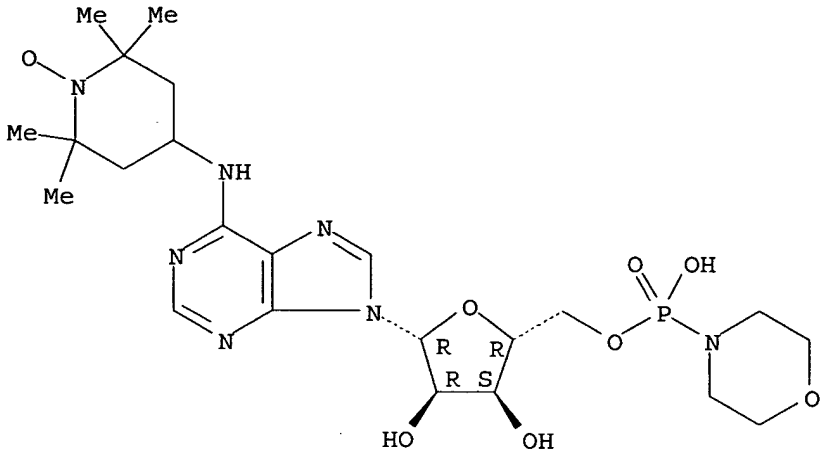


IT **132439-11-3**
(reaction of, with pantetheine phosphate)

RN 132439-11-3 HCAPLUS

CN 1-Piperidinyloxy, 4-[[9-[5-O-(hydroxy-4-morpholinylphosphinyl)-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-5 (Enzymes)
IT 132439-09-9P 132439-10-2P **132439-12-4P**
(preparation and hydroxyacyl-CoA-dehydrogenase binding by, coenzyme and substrate spatial arrangement in enzyme active site in relation to)
IT **132439-11-3**
(reaction of, with pantetheine phosphate)

L22 ANSWER 13 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:590737 HCAPLUS
DOCUMENT NUMBER: 111:190737
TITLE: Spin-labeled analogs of ATP, ADP and AMP: substitutes for normal nucleotides in biochemical systems
AUTHOR(S): Ubom, Gregory A.; Hunt, John B.; Timmons, R. B.
CORPORATE SOURCE: Fac. Med. Sci., Univ. Jos, Jos, Nigeria
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1989), 997(1-2), 1-8
CODEN: BBAEDZ; ISSN: 0167-4838
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The different roles and effectiveness of adenosine monophosphate, diphosphate, and triphosphate labeled at the 6 position of the purine ring with 2,2,6,6-tetramethylpiperidine-1-oxyl in reactions catalyzed by Escherichia coli glutamine synthetase have been investigated. The spin-labeled ATP (Tempo-ATP) serves as a substrate in the glutamine synthesis reaction and in the adenylation of E. coli glutamine synthetase catalyzed by ATP: glutamine adenylyl transferase with essentially the same effectiveness as normal ATP. In another reaction (γ-glutamyltransferase), Tempo ADP serves as an effector with a Km of 9.4 + 10-8M compared to 1.2 + 10-8M for the normal ADP, while covalently bonded Tempo-AMP serves as a modifier on the catalytic properties of E. coli glutamine synthetase just as the covalently bonded normal AMP does. The dissociation consts. between the labeled nucleotides, Mn2+, Mg2+, and Ca2+ are in the same order of magnitude as the binding consts. for

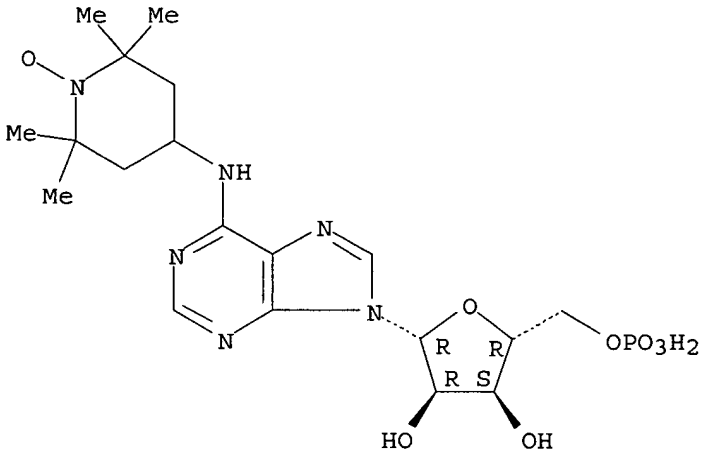
those cations and the corresponding normal nucleotides. Apparently, the spin-labeled nucleotides are good substitutes for the normal nucleotides in the biochem. systems studied.

IT **54187-54-1P**
(preparation and phosphorylation of, as substitute for normal nucleotides)

RN 54187-54-1 HCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

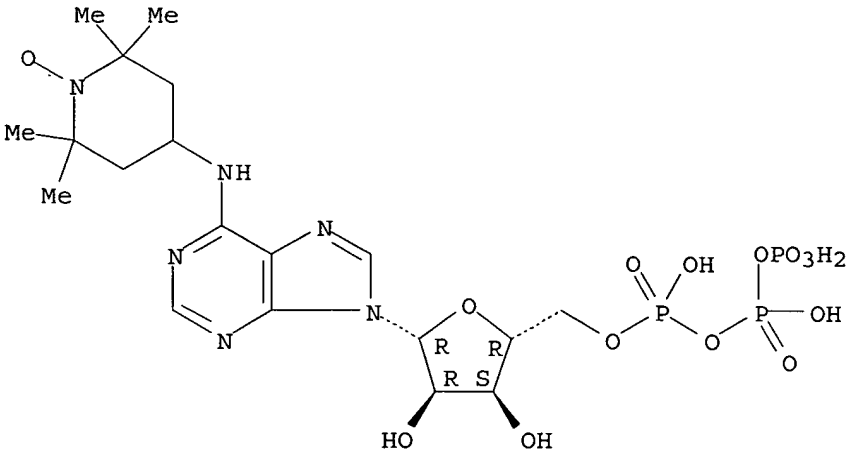


IT **33913-54-1P**, Tempo-ATP **61468-67-5P**
(preparation of, as substitute for normal nucleotide)

RN 33913-54-1 HCAPLUS

CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

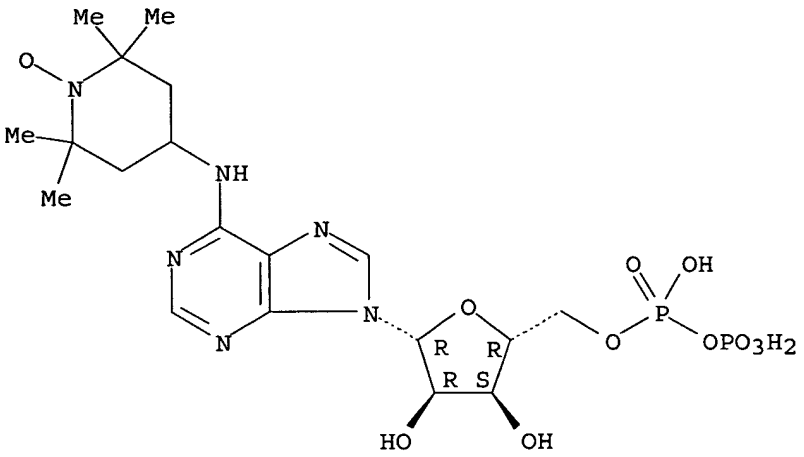


RN 61468-67-5 HCAPLUS

CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 9-5 (Biochemical Methods)
Section cross-reference(s): 7

IT **54187-54-1P**
(preparation and phosphorylation of, as substitute for normal nucleotides)

IT **33913-54-1P**, Tempo-ATP **61468-67-5P**
(preparation of, as substitute for normal nucleotide)

L22 ANSWER 14 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:569915 HCAPLUS
DOCUMENT NUMBER: 111:169915
TITLE: Catalytic mechanism and interactions of NAD+ with glyceraldehyde-3-phosphate dehydrogenase: correlation of EPR data and enzymic studies
AUTHOR(S): Wilder, Robert T.; Venkataramu, S. D.; Dalton, Larry R.; Birktoft, Jens J.; Trommer, Wolfgang E.; Park, Jane H.
CORPORATE SOURCE: Dep. Mol. Physiol., Vanderbilt Univ., Nashville, TN, USA
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1989), 997(1-2), 65-77
CODEN: BBAEDZ; ISSN: 0167-4838
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Perdeuterated spin label (DSL) analogs of NAD, with the spin label attached at either the C8 or N6 position of the adenine ring, were employed in an EPR investigation of models for neg. cooperativity of coenzyme binding to tetrameric glyceraldehyde 3-phosphate dehydrogenase and conformational changes of the DSL-NAD-enzyme complex during the catalytic reaction. C8-DSL-NAD and N6-DSL-NAD showed 80 and 45% of the activity of the native NAD, resp. Therefore, these spin-labeled compds. are very efficacious for investigations of the motional dynamics and catalytic mechanism of this dehydrogenase. Perdeuterated spin labels enhanced spectral sensitivity and resolution, thereby enabling the simultaneous detection of spin-labeled NAD in 3 conditions: (1) DSL-NAD freely tumbling in the presence of, but not bound to, glyceraldehyde

3-phosphate dehydrogenase, (2) DSL-NAD tightly bound to enzyme subunits remote (58 Å) from other NAD binding sites, and (3) DSL-NAD bound to adjacent monomers and exhibiting electron dipolar interactions (8-9 or 12-13 Å, depending on the analog). Detns. of relative amts. of DSL-NAD in these 3 environments and measurements of the binding consts., K1-K4, permitted characterization of the math. model describing the neg. cooperativity in the binding of 4 NAD to glyceraldehyde 3-phosphate dehydrogenase. For enzyme crystallized from rabbit muscle, EPR results were consistent with the ligand-induced sequential model and inconsistent with the pre-existing asymmetry models. The electron dipolar interaction observed between spin labels bound to 2 adjacent glyceraldehyde 3-phosphate dehydrogenase monomers (8-9 or 12-13 Å) related by the R-axis provided a sensitive probe of conformational changes of the enzyme-DSL-NAD complex. When glyceraldehyde 3-phosphate was covalently bound to the active site cysteine-149, an increase in electron dipolar interaction was observed This increase was consistent with a closer approximation of spin labels produced by steric interactions between the phosphoglyceryl residue and DSL-NAD. Coenzyme reduction (DSL-NADH) or inactivation of the dehydrogenase by carboxymethylation of the active site cysteine-149 did not produce changes in the dipolar interactions of spatial separation of the spin labels attached to the adenine moiety of the NAD. However, coenzyme reduction or carboxymethylation did alter the stoichiometry of binding and caused the release of approx. one loosely bound DSL-NAD from the enzyme. These findings suggest ionic charge interactions are important in coenzyme binding at the active site.

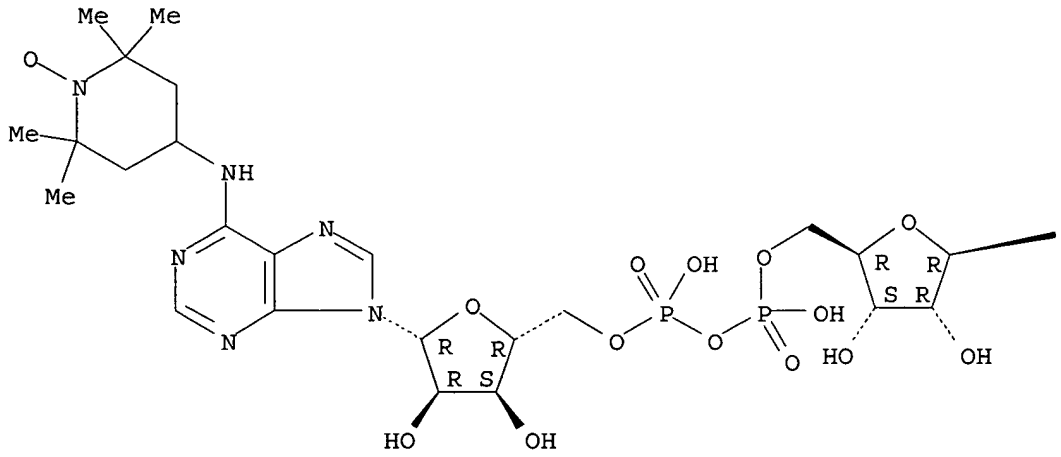
IT **123253-08-7 123277-36-1**
(glyceraldehyde phosphate dehydrogenase binding by, other NAD spin label analog comparison with)

RN 123253-08-7 HCAPLUS

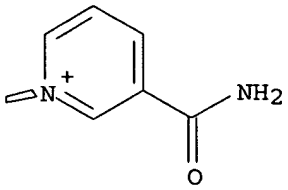
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



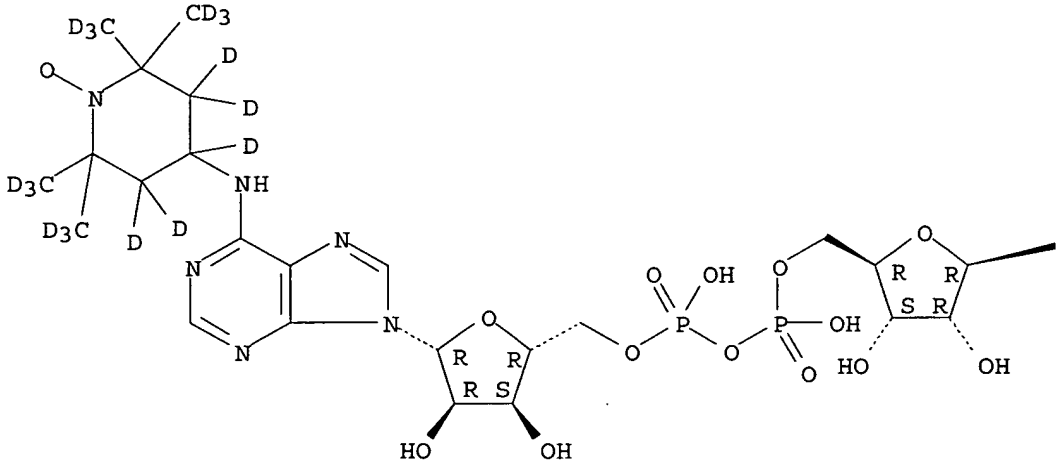
PAGE 1-B



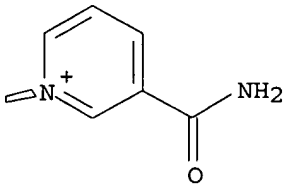
RN 123277-36-1 HCAPLUS
CN 1-Piperidinyl-3,3,4,5,5-d5-oxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetra(methyl-d3)-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

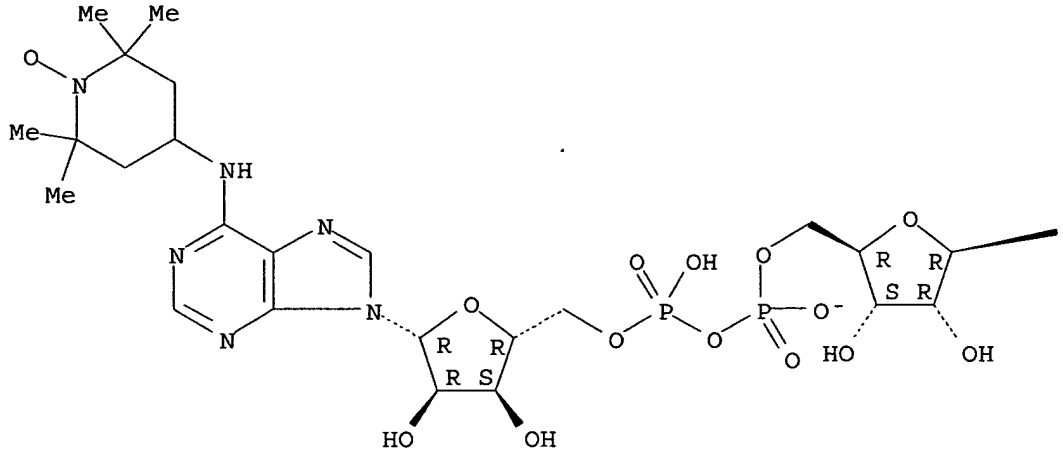


CC 7-3 (Enzymes)
IT **123253-08-7 123277-36-1** 123277-37-2
(glyceraldehyde phosphate dehydrogenase binding by, other NAD spin label analog comparison with)

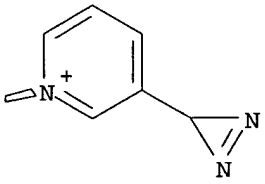
L22 ANSWER 15 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:419841 HCAPLUS
DOCUMENT NUMBER: 107:19841
TITLE: Synthesis of spin-labeled photoaffinity derivatives of NAD+ and their interaction with lactate dehydrogenase
AUTHOR(S): Wolf, A.; Fritzsche, T. M.; Rudy, B.; Trommer, W. E.
CORPORATE SOURCE: Fachbereich Chem., Univ. Kaiserslautern, Kaiserslautern, D-6750, Fed. Rep. Ger.
SOURCE: FEBS Letters (1987), 212(2), 203-7
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of NAD derivs. spin-labeled at either N8 or C8 of the adenine ring is described in which the carboxamide function of the nicotinamide moiety is replaced by a diazirine ring. Irradiation of these compds. at 350 nm generates a carbene which will react with any functional group in its vicinity including hydrocarbons. Both NAD derivs. form tight ternary complexes with lactate dehydrogenase and were covalently incorporated into this enzyme. They may be employed for ESR studies when noncovalent interactions are too weak for motionally restricted species to be observed
IT **108904-97-8P**
(preparation and lactate dehydrogenase photoaffinity labeling with)
RN 108904-97-8 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(3H-diazirin-3-yl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



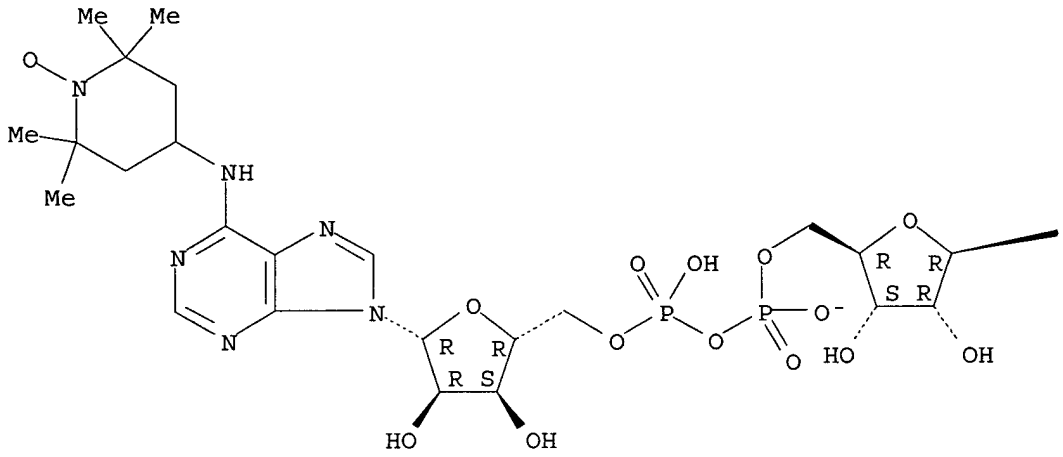
PAGE 1-B



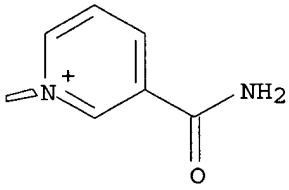
IT **61468-69-7**
(reaction of, with diazirinylpyridine in NAD glycohydrolase presence)
RN 61468-69-7 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
Section cross-reference(s): 9, 33
IT **108904-97-8P** 108904-98-9P
(preparation and lactate dehydrogenase photoaffinity labeling with)
IT **61468-69-7** 63958-39-4
(reaction of, with diazirinylpyridine in NAD glycohydrolase presence)

L22 ANSWER 16 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:420875 HCAPLUS
DOCUMENT NUMBER: 105:20875
TITLE: Binding of nicotinamide nucleotides to dihydrolipoamide dehydrogenase measured with spin-labeled analogs
AUTHOR(S): Schrenk, Dieter F.; Bisswanger, Hans
CORPORATE SOURCE: Physiol.-Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.
SOURCE: Journal of Protein Chemistry (1985), 4(4), 227-34
CODEN: JPCHD2; ISSN: 0277-8033
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Binding of NAD and NADH to dihydrolipoamide dehydrogenase from Escherichia coli and from pig heart was measured by using the spin-labeled analogs N6-(2,2,6,6-tetramethylpiperidine-4-yl-1-oxyl)-NAD and -NADH. A decrease in the peak amplitudes of the resp. EPR spectra results after adding enzyme to the cofactor analogs. With the bacterial enzyme, normal hyperbolic saturation behavior with the NAD analog and 1 binding site per subunit [Ks (dissociation constant) = 0.51 mM] are observed, whereas the NADH analog reveals a sigmoidal binding characteristic. A high-affinity and a low-affinity site (Ks = 0.087 and 0.33 mM, resp.) are found for binding of the NAD analog to the pig heart enzyme, and only 1 type of binding site is observed for the NADH analog (Ks = 22 μM).

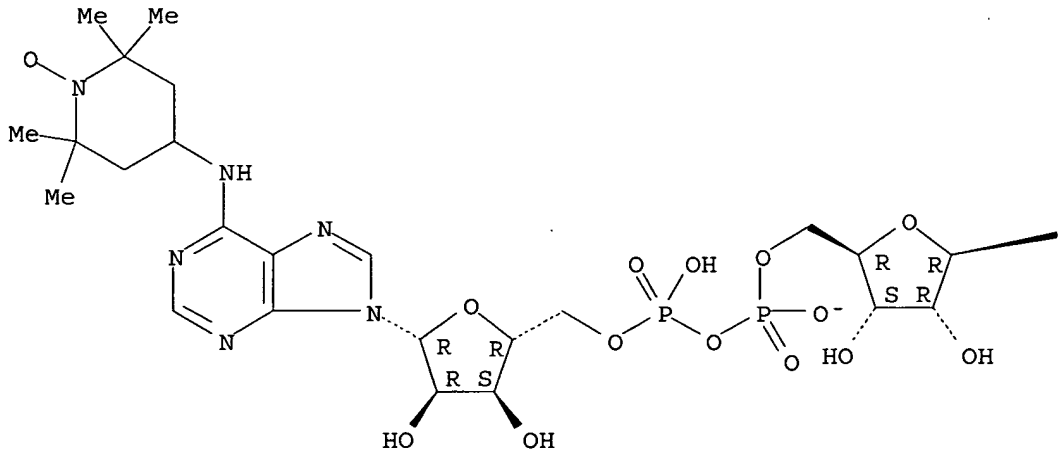
IT **61468-69-7 72548-71-1**
(dihydrolipoamide dehydrogenase of Escherichia coli and pig heart binding of, kinetics of)

RN 61468-69-7 HCAPLUS

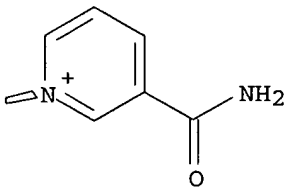
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



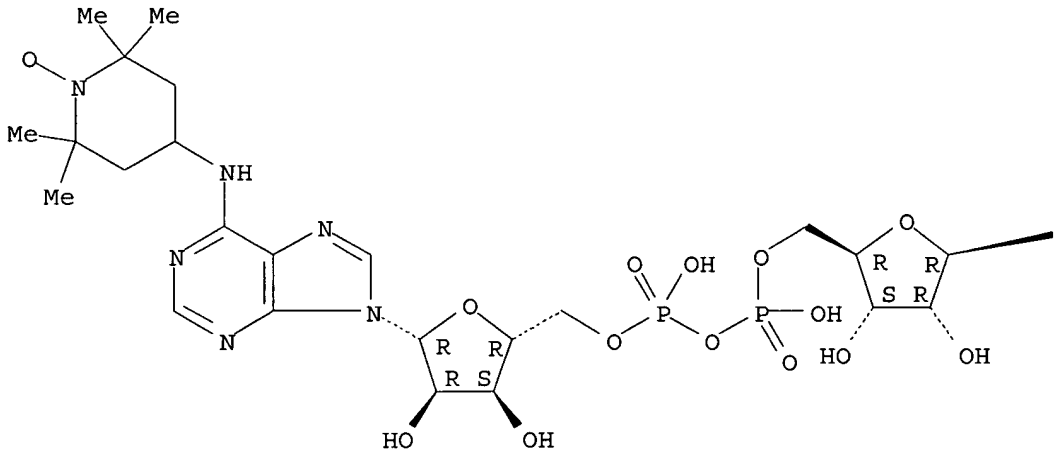
PAGE 1-B



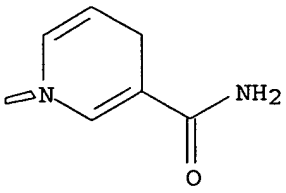
RN 72548-71-1 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-pyridinecarboxamide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
IT **61468-69-7 72548-71-1**
(dihydrolipoamide dehydrogenase of Escherichia coli and pig heart binding of, kinetics of)

L22 ANSWER 17 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:74649 HCAPLUS
DOCUMENT NUMBER: 102:74649
TITLE: Complex formation between nucleotides and D-β-hydroxybutyrate dehydrogenase studied by fluorescence and EPR spectroscopy
AUTHOR(S): Fritzsche, Thomas M.; McIntyre, J. Oliver; Fleischer, Sidney; Trommer, Wolfgang E.
CORPORATE SOURCE: Inst. Org. Chem. Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1984), 791(2), 173-85
CODEN: BBAEDZ; ISSN: 0167-4838
DOCUMENT TYPE: Journal
LANGUAGE: English
AB D-β-Hydroxybutyrate dehydrogenase (EC 1.1.1.30) (I) is a lipid-requiring enzyme which specifically requires phosphatidylcholine (PC) for enzymic activity. The PC modifies the binding and orientation of the coenzyme, NAD(H), with respect to the enzyme. In the present study, 2 derivs. of NAD, spin-labeled either at N-6 or C-8 of the adenine ring, were found to be active as coenzyme. The binding affinity of NADH to I was optimized by increasing the salt concentration and increasing the pH from 6 to 8, with the pK at 6.8. Monomethylmalonate, a substrate analog, enhanced NADH binding. Sulfite strongly enhanced the binding of NAD via the enzyme-catalyzed formation of an adduct of sulfite with the nucleotide; the dissociation constant for binding of NAD-sulfite was in the micromolar range, whereas NAD binding was more than a magnitude weaker. The binding of spin-labeled NAD(H) was further characterized by EPR spectroscopy. Increased sensitivity and resolution were obtained with the use of NAD(H) analogs perdeuterated in the spin-label moiety. For these analogs bound to I in phospholipid vesicles, EPR studies showed the spin-label moiety to be constrained and revealed 2 distinct components. Increasing the viscosity of the medium by addition of glycerol affected the EPR spectral characteristics of only the component with the smaller resolved averaged hyperfine splitting.
IT **61468-69-7**

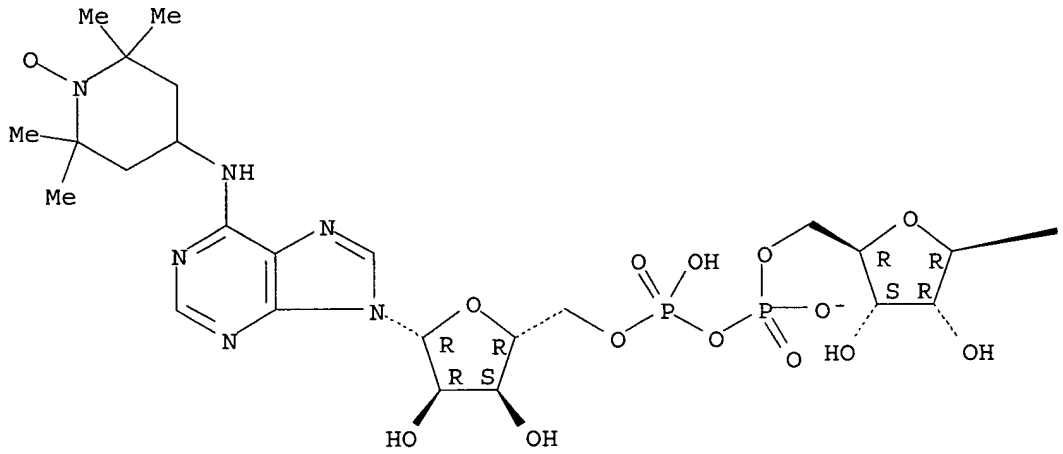
(β-hydroxybutyrate dehydrogenase binding of, kinetics of, ESR and fluorescence in relation to)

RN 61468-69-7 HCAPLUS

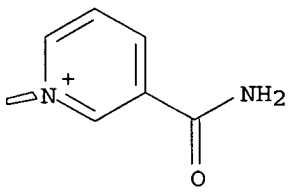
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
Section cross-reference(s): 77

IT **61468-69-7** 63958-39-4
(β-hydroxybutyrate dehydrogenase binding of, kinetics of, ESR and fluorescence in relation to)

L22 ANSWER 18 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:74639 HCAPLUS

DOCUMENT NUMBER: 102:74639

TITLE: The synthesis of nitrogen-15- and deuterium-substituted, spin-labeled analogs of NAD+ and their use in EPR studies of

dehydrogenases

AUTHOR(S): Philipp, Reinhard; McIntyre, J. Oliver; Robinson, Bruce H.; Huth, Helga; Trommer, Wolfgang; Fleischer, Sidney

CORPORATE SOURCE: Dep. Chem., Univ. Kaiserslautern, Kaiserslautern, Fed. Rep. Ger.

SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1984), 790(3), 251-8
CODEN: BBAEDZ; ISSN: 0167-4838

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two spin-labeled analogs of NAD+ were synthesized with a 15N-labeled and perdeuterated nitroxide radical, 4-amino-2,2,6,6-[2H17,15N]tetramethylpiperidone-1-oxyl, which was attached to either the C-6 or C-8 position of the purine ring. The EPR spectra of these derivs. exhibit an .apprx.6-fold increase in sensitivity compared with the corresponding 14N, protonated analogs due to a decrease in both the number of nuclear manifolds (from 3 to 2) and the linewidth. In enhanced spectral resolution obtained with (2H17,15N)spin-labeled-NAD+ analogs has facilitated simulation of the EPR lineshape of the nucleotide bound to lactate dehydrogenase (EC 1.1.1.27). The spin-label moiety exhibits highly constrained motion indicative of a single environment. The motion of the spin label does not reflect the overall motion of the enzyme; rather, it is characteristic of some limited mobility relative to the lactate dehydrogenase. By contrast, the spin label on the membrane-bound enzyme D-β-hydroxybutyrate dehydrogenase (EC 1.1.1.30) is completely immobilized and exhibits 2 distinct spectral components for spin-labeled NAD+, which appear to differ in the polarity of the environment of the nitroxide.

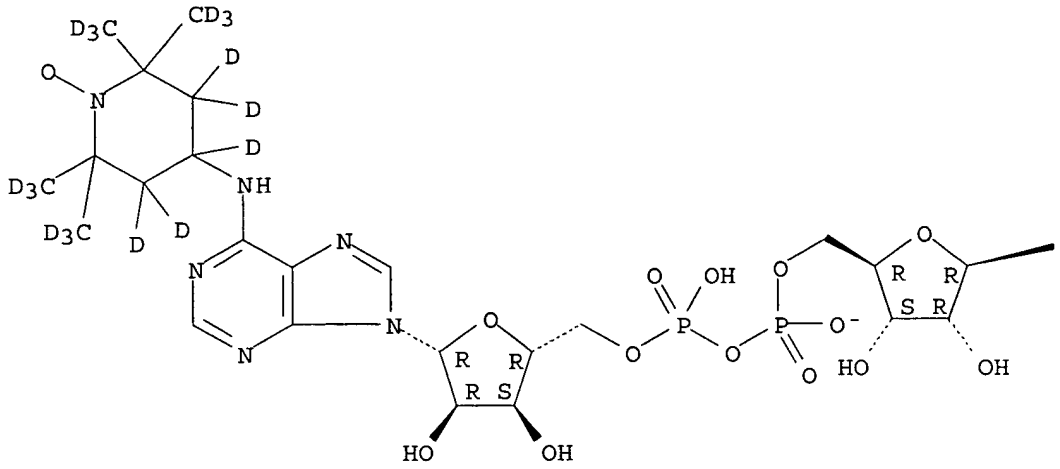
IT **81403-89-6**
(in dehydrogenase characterization by ESR)

RN 81403-89-6 HCAPLUS

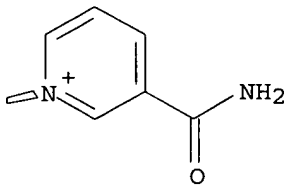
CN 1-Piperidinyl-3,3,4,5,5-d5-oxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetra(methyl-d3)-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



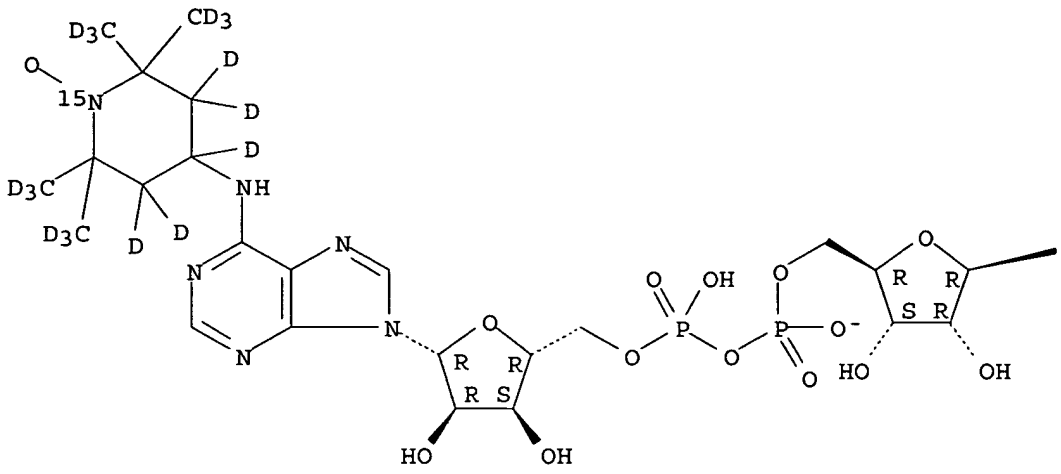
PAGE 1-B



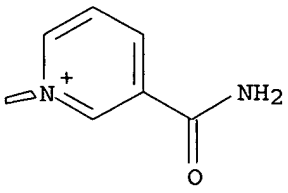
IT **92387-76-3P**
(preparation and use in dehydrogenase characterization by ESR)
RN 92387-76-3 HCAPLUS
CN 1-Piperidinyl-3,3,4,5,5-d5-1-15N-oxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetra(methyl-d3)-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
Section cross-reference(s): 77
IT 53-84-9D, spin-labeled derivs. **81403-89-6** 81403-90-9
(in dehydrogenase characterization by ESR)
IT **92387-76-3P** 94704-72-0P
(preparation and use in dehydrogenase characterization by ESR)

L22 ANSWER 19 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:566234 HCAPLUS
DOCUMENT NUMBER: 101:166234
TITLE: Interactions and spatial arrangement of spin-labeled NAD+ bound to glyceraldehyde-3-phosphate dehydrogenase. Comparison of EPR and x-ray modeling data
AUTHOR(S): Beth, Albert H.; Robinson, Bruce H.; Cobb, Charles E.; Dalton, Larry R.; Trommer, Wolfgang E.; Birktoft, Jens J.; Park, Jane H.
CORPORATE SOURCE: Dep. Physiol., Vanderbilt Univ., Nashville, TN, 37232, USA
SOURCE: Journal of Biological Chemistry (1984), 259(15), 9717-28

CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The spatial arrangement of NAD in remote and adjacent binding sites in various stoichiometric complexes with tetrameric glyceraldehyde 3-phosphate dehydrogenase from rabbit muscle was examined via EPR spectroscopy. An adenosine N6-15N,2H17 spin-labeled derivative of NAD (SL-NAD) was chemical synthesized for this work. The spectral simplifications and narrow line widths afforded by 15N and 2H substitution enabled exptl. EPR spectra to be deconvoluted into their 3 component spectra: (1) unbound coenzyme, (2) bound coenzyme without adjacent site occupied, and (3) bound coenzyme with adjacent site occupied. The binding of SL-NAD in adjacent active centers of R axis-related subunits resulted in resolved dipolar interactions which characterized intersubunit distances. Binding to distant subunits related by the P and Q axes gave no dipolar interaction. Once the 1st NAD site was occupied, EPR spectra at various stoichiometries provided evidence for nonpreferential spatial binding of SL-NAD to the three unoccupied sites. EPR spectral simulations indicated a separation of 12.8 Å for the unpaired electrons of spin label moieties of R axis-related coenzymes. Mol. modeling based on x-ray crystallog. data predicted 11-13 Å. The angles and distance relating to interacting spin-labels were calculated from atomic coordinates based on mol. modeling of both anti-anti and anti-syn (adenine-ribose) conformations of SL-NAD. Computer-generated line-shapes indicated best agreement with exptl. EPR results when the anti-anti geometry was employed. Comparison of EPR spectra from soluble and ammonium sulfate-precipitated enzymes indicated that the NAD-binding domains are positioned equivalently in the 2 phys. states. Since the observed dipolar line-shapes were critically dependent on the distance and geometry relating to the interacting SL-NAD, these data provided direct evidence for a high degree of conservation of quaternary structure of the enzyme in the hydrated crystalline state. Studies on the enzyme isolated from human erythrocytes also indicated a close correlation with the rabbit muscle enzyme in both the arrangement of NAD-binding domains and neg. cooperativity of coenzyme binding.

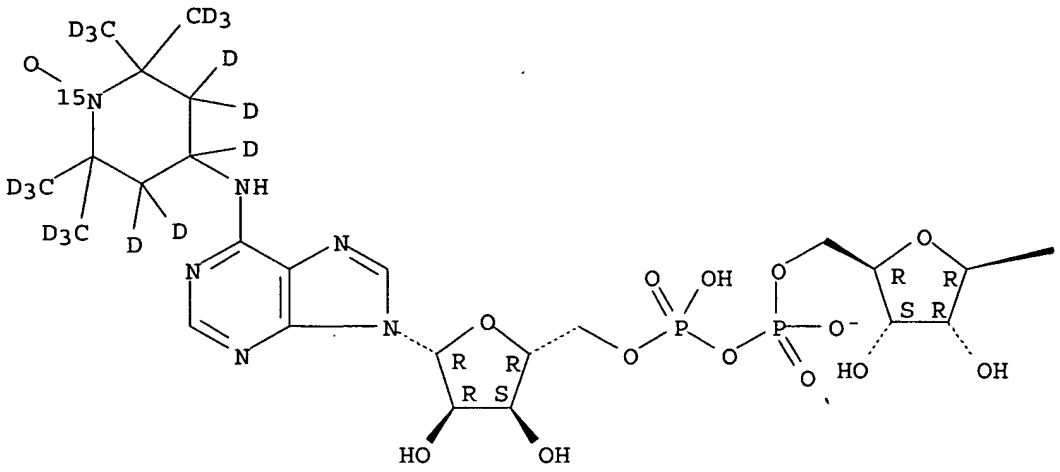
IT **92387-76-3**
(glyceraldehyde phosphate dehydrogenase binding of, ESR study of)

RN 92387-76-3 HCAPLUS

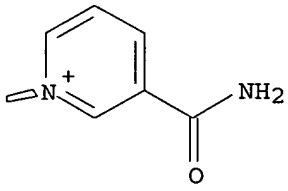
CN 1-Piperidinyl-3,3,4,5,5-d5-1-15N-oxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetra(methyl-d3)-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-5 (Enzymes)
IT **92387-76-3**
(glyceraldehyde phosphate dehydrogenase binding of, ESR study of)

L22 ANSWER 20 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:611461 HCAPLUS
DOCUMENT NUMBER: 97:211461
TITLE: Structure-function relationship in the allosteric L-lactate dehydrogenases from Lactobacillus casei and Lactobacillus curvatus
AUTHOR(S): Mayr, Ulrich; Hensel, Reinhard; Deparade, Matthias; Pauly, Hans E.; Pfleiderer, Gerhard; Trommer, Wolfgang E.
CORPORATE SOURCE: Bot. Inst., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: European Journal of Biochemistry (1982), 126(3), 549-58
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The activation of the allosteric L-lactate dehydrogenases from L. casei and L. curvatus induced by binding of the effectors fructose 1,6-diphosphate (I) and Mn2+ is correlated with conformational changes as indicated by alterations of the tryptophan and tyrosine absorption and by an alteration of the tryptophan fluorescence of the proteins. Both enzymes contain 4 NADH- and I-binding sites/tetramer as determined by fluorescence measurements. In the case of the L. casei enzyme ≥4 Mn2+-binding sites were determined for the tetrameric state by ESR spectroscopy. The modification of tryptophan of the L. casei enzyme with dimethyl-(2-hydroxy-5-nitrobenzyl)sulfonium bromide suggests that the alteration of the tryptophan absorption is due to a tryptophan residue being located in the interior of the protein, whereas the alteration of the tryptophan fluorescence is due to a 2nd tryptophan residue which is located on the surface of the enzyme. Thus, the effector-induced conformational changes may cause structural alterations in an inner as well as in the outer region. To obtain information about the distance between the coenzyme and Mn2+-binding sites, ESR spectra were recorded of the spin-labeled NADH analogs bound to the L. casei enzyme in the presence and absence of Mn2+. The analogs were substituted at C-6 or C-8 with a 4-(2,2,6,6-tetramethyl-piperidinyl-1-oxyl)-amino group. The oxidized forms of both derivs., labeled by a nitroxide radical, were active coenzymes. However, no spin-spin interaction between the spin label and Mn2+ could be observed, indicating that the Mn2+-binding site is >1.5-2.0 nm apart from the adenine moiety of the coenzyme. Although a direct interaction between the metal and coenzyme is unlikely because of this large distance, binding of the effectors to the L. casei enzyme causes changes of the fluorescence of enzyme-bound NADH. Thus, the bound coenzyme appears to be affected by the conformational changes in the L. casei L-lactate dehydrogenase induced by I and Mn2+.

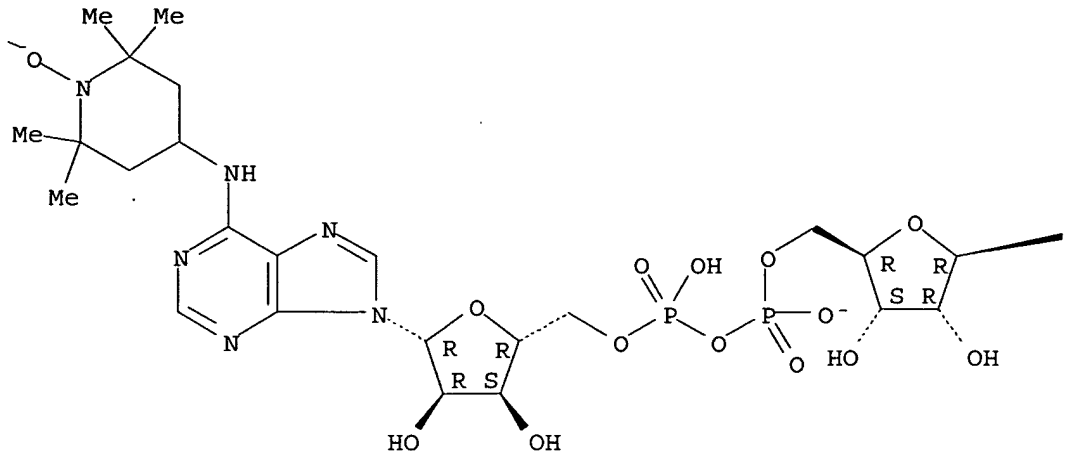
IT **61468-69-7**
(lactate dehydrogenase of Lactobacillus binding of, conformation in relation to)

RN 61468-69-7 HCAPLUS

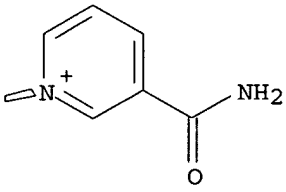
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



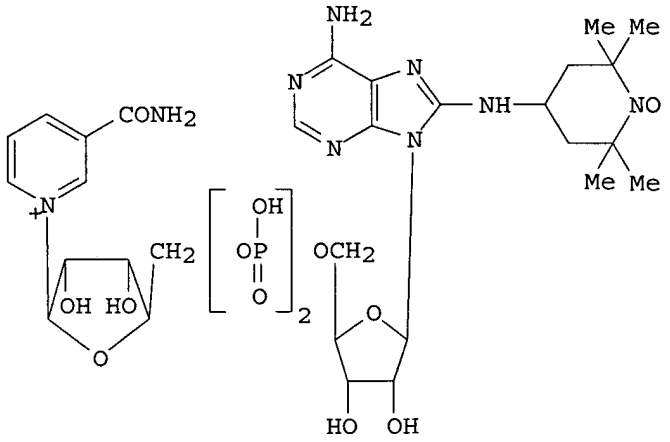
PAGE 1-B



CC 7-5 (Enzymes)
IT 58-68-4 488-69-7 7439-96-5, reactions **61468-69-7**
63958-39-4
(lactate dehydrogenase of Lactobacillus binding of, conformation in relation to)

L22 ANSWER 21 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:595013 HCAPLUS
DOCUMENT NUMBER: 97:195013
TITLE: The role of the nicotinamide moiety of NAD+ for negative cooperativity in glyceraldehyde-3-phosphate dehydrogenase as studied by spin-labeled cofactors
AUTHOR(S): Gloeggler, Klaus G.; Balasubramanian, K.; Beth, Albert H.; Park, Jane H.; Trommer, Wolfgang E.
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1982),

706(2), 197-202
CODEN: BBAEDZ; ISSN: 0167-4838
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Two derivs. of NAD spin-labeled at N6 or C-8 (I) of the adenine ring are active coenzymes of glyceraldehyde 3-phosphate dehydrogenase (EC 1.2.1.12). When >2 equiv of either spin-labeled NAD are bound to the tetrameric enzyme, spin-spin interaction is observed in the ESR spectra. After reduction of enzyme-bound I to the corresponding NADH derivative, the addnl. peaks due to this spin-spin interaction disappear, which implies that the distance between the 2 radicals increases. Apparently, the coenzyme slides further towards the active site on reduction ADP-ribose spin-labeled at C-8 binds noncooperatively, exhibiting a dissociation constant of 33 μM. Even with 3.5 equiv bound to the enzyme, spin-spin interaction is not observed AMP spin-labeled at C-8 combines with 2 sites/monomer, or a total of 8/tetramer. The resp. dissociation consts. are 30 μM and 2.3 mM. Phosphate competes with AMP bound to the weak site; spin-spin interaction is not observed ATP spin-labeled at C-8 is bound .apprx.10-fold tighter than the corresponding AMP derivative Four equivs. of ATP are bound per tetramer, but it exhibits no spin-spin interaction. The structure of the pyridine moiety of the coenzymes plays a role in orienting the adenine ring and, thus, affects the cooperativity. The N6 derivative of NAD also shows spin-spin interaction; however, only data for the C-8 derivs. are shown in detail.

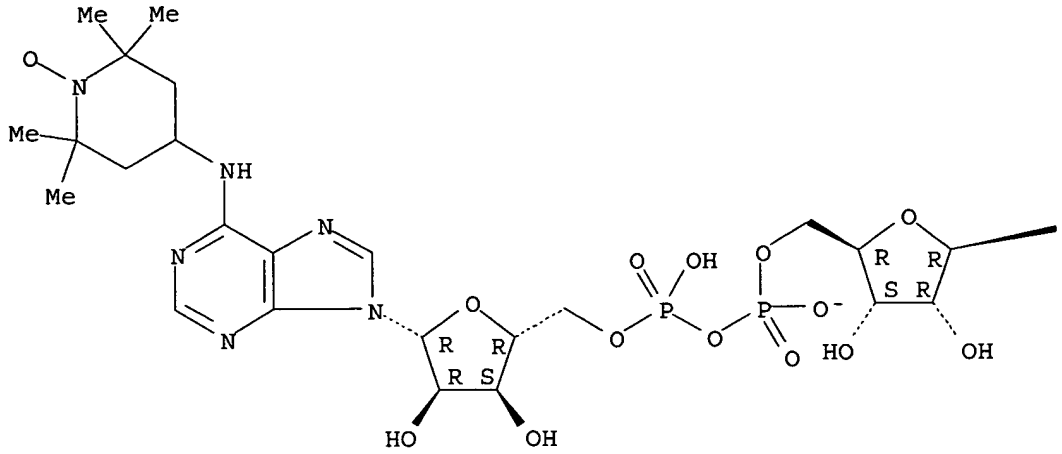
IT **61468-69-7**
(glyceraldehyde phosphate dehydrogenase interaction with, ESR of, neg. cooperativity in relation to)

RN 61468-69-7 HCAPLUS

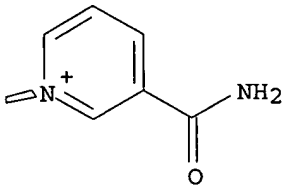
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
IT **61468-69-7** 63958-39-4
(glyceraldehyde phosphate dehydrogenase interaction with, ESR of, neg. cooperativity in relation to)

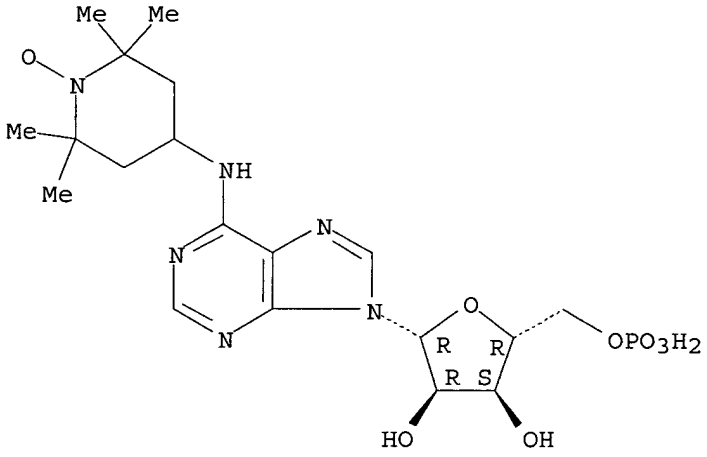
L22 ANSWER 22 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:158087 HCAPLUS
DOCUMENT NUMBER: 96:158087
TITLE: The synthesis of deuterium-substituted, spin-labeled analogs of AMP and NAD+ and their use in ESR studies of lactate dehydrogenase
AUTHOR(S): Gloeggler, Klaus G.; Balasubramanian, K.; Beth, Albert; Fritzsche, Thomas M.; Park, Jane H.; Pearson, Donald E.; Trommer, Wolfgang E.; Venkataramu, Sindhagatta D.
CORPORATE SOURCE: Dep. Physiol., Vanderbilt Univ., Nashville, TN, USA
SOURCE: Biochimica et Biophysica Acta, Protein Structure and Molecular Enzymology (1982), 701(2), 224-8
CODEN: BBAEDZ; ISSN: 0167-4838

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two spin-labeled analogs of AMP and NAD were synthesized, in which a perdeuterated nitroxide radical (4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl) was attached to the C-6 or C-8 position of the adenine ring. The ESR spectra of these derivs. exhibited a 4-fold increase in sensitivity and a concomitant decrease in linewidth as compared to the corresponding protonated analogs. The improved resolution of composite spectra consisting of freely tumbling and immobilized components was demonstrated in ternary complexes of the spin-labeled NAD derivs. with lactate dehydrogenase (EC 1.1.1.27) and oxalate.

IT **54187-54-1**
(ESR of)
RN 54187-54-1 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

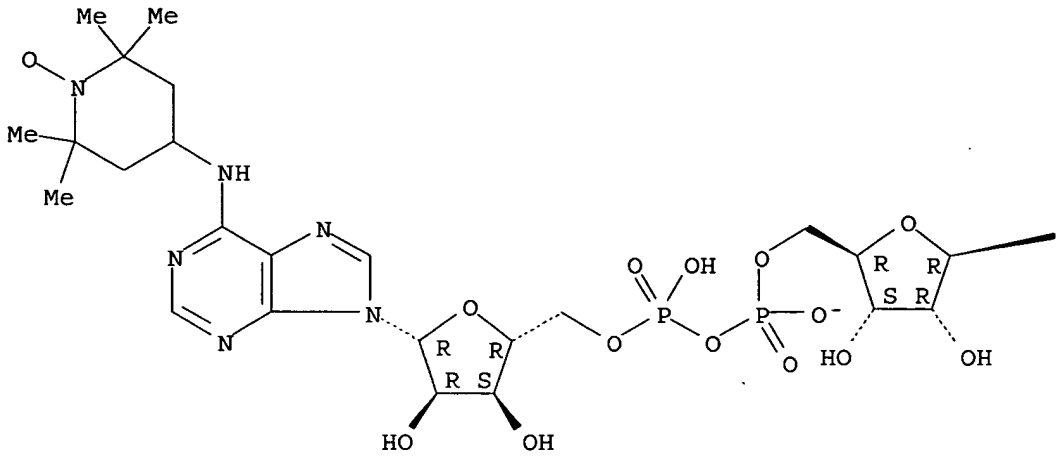
Absolute stereochemistry.



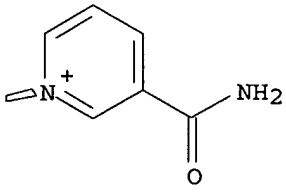
IT **61468-69-7**
(ESR of, lactate dehydrogenase binding in relation to)
RN 61468-69-7 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



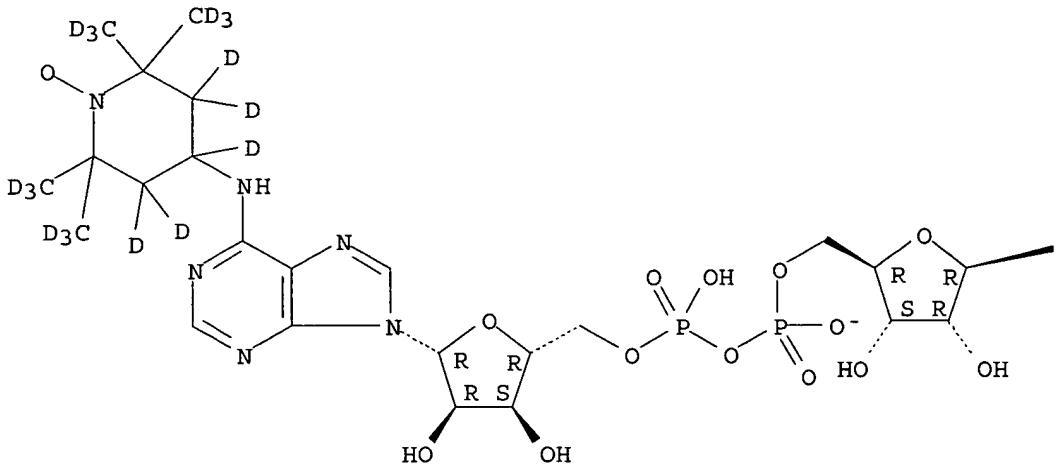
PAGE 1-B



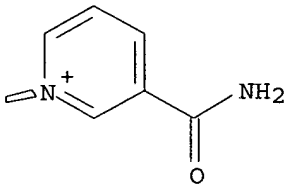
IT **81403-89-6P**
(preparation and ESR of, lactate dehydrogenase binding in relation to)
RN 81403-89-6 HCAPLUS
CN 1-Piperidinyl-3,3,4,5,5-d5-oxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetra(methyl-d3)-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

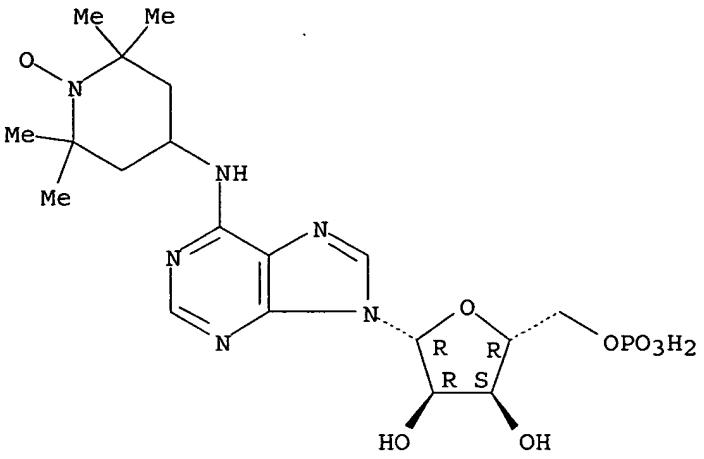


PAGE 1-B



IT **54187-54-1P**
(preparation and condensation with NMN)
RN 54187-54-1 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
IT **54187-54-1** 63958-40-7
(ESR of)
IT **61468-69-7** 63958-39-4
(ESR of, lactate dehydrogenase binding in relation to)
IT **81403-89-6P** 81403-90-9P
(preparation and ESR of, lactate dehydrogenase binding in relation to)
IT **54187-54-1P** 81403-91-0P
(preparation and condensation with NMN)

L22 ANSWER 23 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:48167 HCAPLUS
DOCUMENT NUMBER: 96:48167
TITLE: Synthesis and preliminary biochemical characterization of spin-labeled derivatives of ATP and its 'non-cleavable' analog, adenosine 5'-β,γ-methylenetriphosphate
AUTHOR(S): Gloeggler, Klaus G.; Fritzsche, Thomas M.; Huth, Helga; Trommer, Wolfgang E.
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000, Fed. Rep. Ger.
SOURCE: Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie (1981), 362(11), 1561-5
CODEN: HSZPAZ; ISSN: 0018-4888
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Spin-labeled derivs. were prepared of ATP and its non-cleavable analog β,γ-methylene-ATP, in which 4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl was linked to N-6 or C-8 of the purine ring by its amino group. The triphosphates were active substrates for yeast hexokinase, with Vmax .apprx.70% of the value for ATP. Thus, the bulky spin-label did not significantly alter the enzyme-substrate interaction. In contrast, the corresponding methylene-ATP derivs. were virtually inactive. Substitution of the bridge O by the CH2 group in the triphosphate moiety may prevent analog binding to certain ATP-cleaving enzymes. Binding of spin-labeled ATP and derivs. to D-glyceraldehyde-3-phosphate dehydrogenase and the Ca2+ pump from sarcoplasmic reticulum also

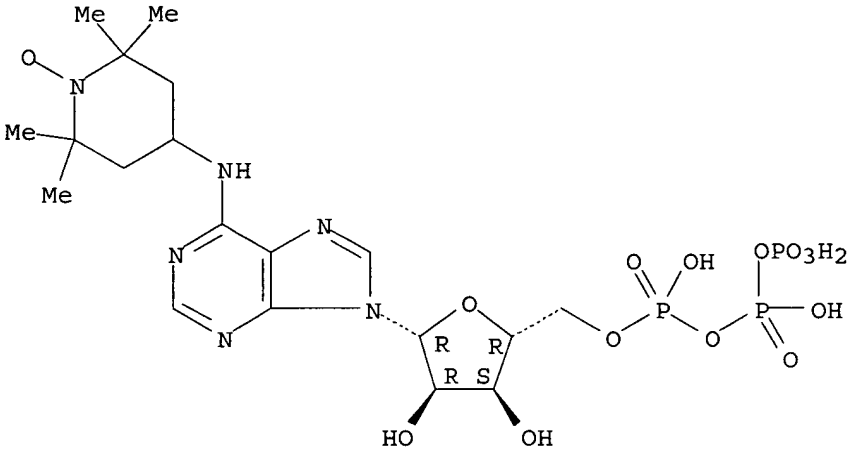
were studied. ESR may be a useful tool in the study of ligand-induced conformational changes in enzymes.

IT **33913-54-1P 80538-65-4P**
(preparation and biol. activity of ATP in relation to)

RN 33913-54-1 HCAPLUS

CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

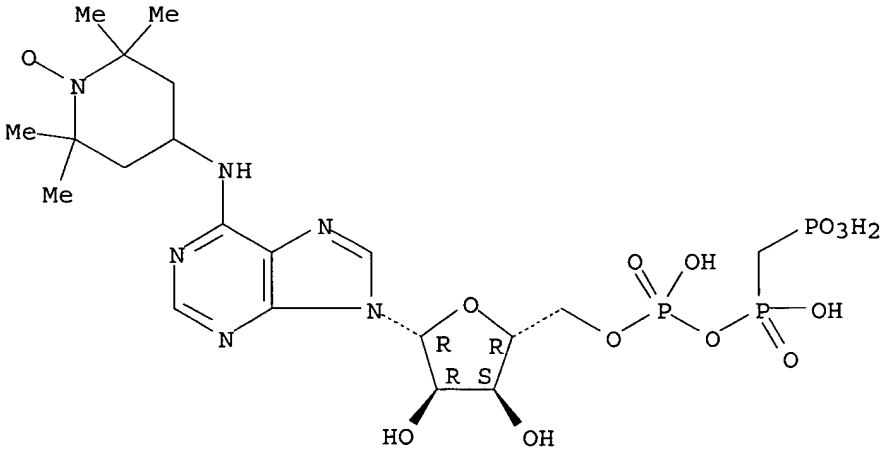
Absolute stereochemistry.



RN 80538-65-4 HCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-[5-O-(1,3,5,5-tetrahydroxy-1,3,5-trioxido-2-oxa-1,3,5-triphosphapent-1-yl)-β-D-ribofuranosyl]-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)
Section cross-reference(s): 33

IT **33913-54-1P** 80538-64-3P **80538-65-4P**
80538-66-5P
(preparation and biol. activity of ATP in relation to)

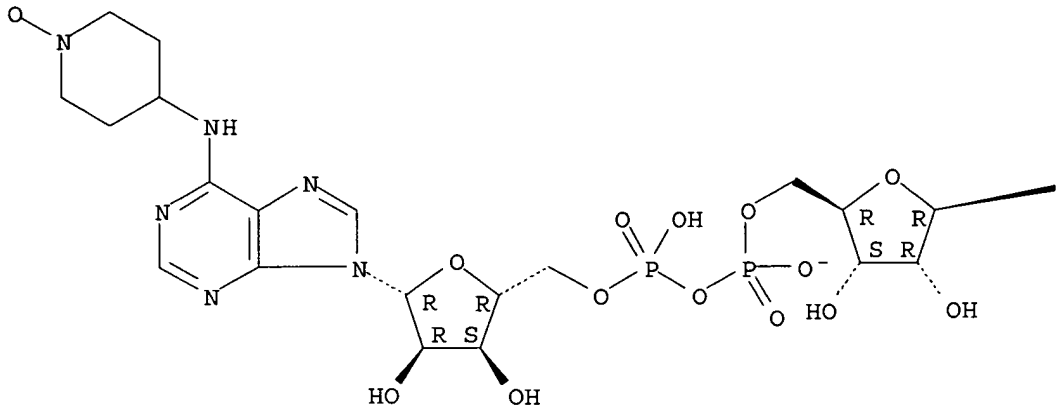
L22 ANSWER 24 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:492828 HCAPLUS
DOCUMENT NUMBER: 95:92828
TITLE: Isolation and properties of glyceraldehyde-3-phosphate dehydrogenase from a sturgeon from the Caspian Sea and its interaction with spin-labeled NAD+ derivatives
AUTHOR(S): Deparade, Matthias P.; Gloeggler, Klaus; Trommer, Wolfgang E.
CORPORATE SOURCE: Inst. Org. Chem. Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Enzymology (1981), 659(2), 422-33
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Glyceraldehyde phosphate dehydrogenase (EC 1.2.1.12) (I) was isolated from the muscle of the sturgeon, Huso huso, from the Caspian Sea. It was closely related to I from the muscle of the Pacific sturgeon, Acipenser transmontanus, with respect to amino acid composition, steady-state kinetics, and coenzyme binding. I of H. huso, as studied by means of a spin-labeled derivative of NAD, was neg. cooperative, exhibiting a Hill coefficient of 0.84 at 12°. Two derivs. of NAD spin-labeled at N6 or C8 of the adenine ring were active coenzymes with Vmax values reaching 35 or 45% of the value for NAD itself. When >2 equiv of either spin-labeled NAD were bound to I, spin-spin interactions were observed in the ESR spectra. Distances between the nitroxide radicals (8-9 Å), calculated from the observed splittings, were in excellent agreement with the data predicted from the crystal structure of the lobster enzyme when the coenzyme is bound in an anti-conformation of the adenine moiety about the glycosidic bond to all 4 subunits.

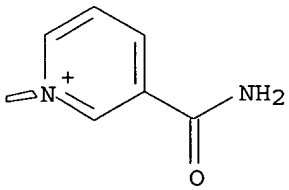
IT **78714-97-3**
(glyceraldehyde phosphate dehydrogenase of sturgeon affinity for)
RN 78714-97-3 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-2 (Enzymes)
IT 78682-53-8 **78714-97-3**
(glyceraldehyde phosphate dehydrogenase of sturgeon affinity for)

L22 ANSWER 25 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:54165 HCAPLUS
DOCUMENT NUMBER: 92:54165
TITLE: Solution conformation of lactate dehydrogenase as studied by saturation transfer ESR spectroscopy
AUTHOR(S): Trommer, Wolfgang E.; Gloeggler, Klaus
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Enzymology (1979), 571(2), 186-94
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Several binary and ternary inhibitor and dead end complexes of pig heart lactate dehydrogenase (EC 1.1.1.27) were studied by saturation transfer ESR spectroscopy using an active NAD analog (N6-(2,2,6,6-tetramethylpiperidin-4-yl-1-oxyl)-NAD. The mobility of the spin-label depended on the nature of small mols. bound at

the remote catalytic end of the coenzyme. The spin-label served as a reporter group monitoring the conformation of the peptide loop that was folded down over the active cleft in crystals of ternary complexes. A fluctuation of the loop between open and closed forms in solution is suggested. The structure of the inhibitor mols. was correlated with their ability to stabilize a more closed conformation of the loop.

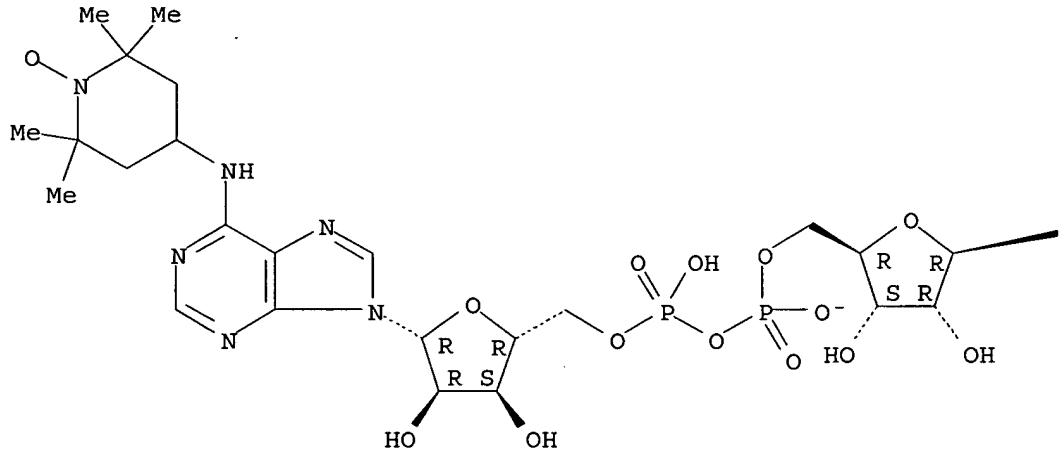
IT **61468-69-7D**, lactate dehydrogenase-inhibitor complexes
72548-71-1D, lactate dehydrogenase-inhibitor complexes
(conformation of, ESR in relation to)

RN 61468-69-7 HCAPLUS

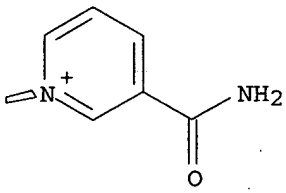
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



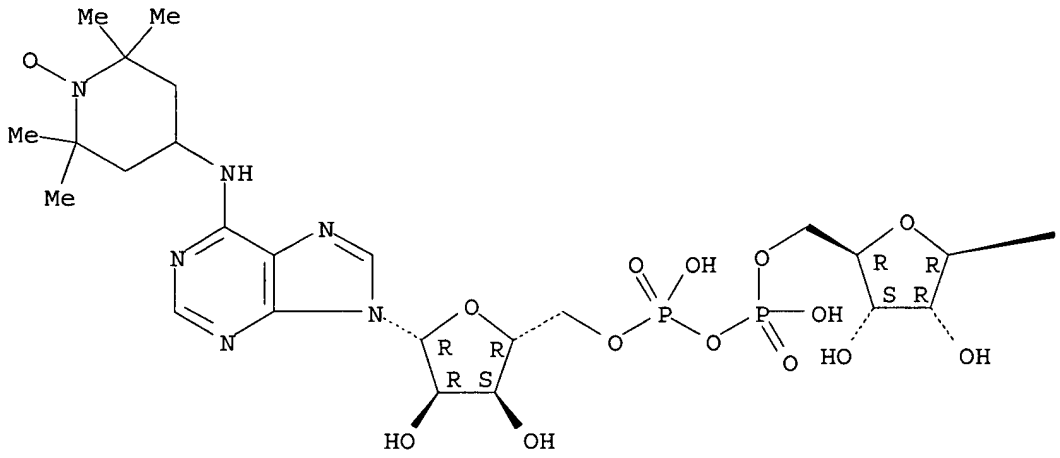
RN 72548-71-1 HCAPLUS

CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-

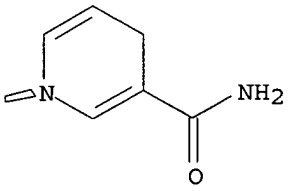
pyridinecarboxamide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-5 (Enzymes)
IT 127-17-3D, spin-labeled lactate dehydrogenase complexes
144-62-7D, spin-labeled lactate dehydrogenase complexes
471-47-6D, spin-labeled lactate dehydrogenase complexes
9001-60-9D, inhibitor complexes 14265-45-3D, spin-labeled lactate dehydrogenase complexes **61468-69-7D**, lactate dehydrogenase-inhibitor complexes **72548-71-1D**, lactate dehydrogenase-inhibitor complexes
(conformation of, ESR in relation to)

L22 ANSWER 26 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:486290 HCAPLUS
DOCUMENT NUMBER: 91:86290
TITLE: Ternary complex formation of pig heart lactate dehydrogenase with spin-labeled coenzymes and inhibitors as studied by electron spin resonance
AUTHOR(S): Wenzel, Herbert R.; Trommer, Wolfgang E.

CORPORATE SOURCE: Abt. Chem., Ruhr-Univ., Bochum, D-4630, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Enzymology (1979), 568(2), 287-96
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The formation of ternary inhibitor and dead-end complexes of pig heart lactate dehydrogenase was studied using 2 NAD derivs., spin-labeled at N6 and C-8 of the adenine ring. Dissociation consts. calculated for the inhibitors oxamate and oxalate from their corresponding ternary complexes are in excellent agreement with data from literature derived from sedimentation expts. However, the recently postulated enzyme-NADH-sulfite complex was not observed The mobility of the spin-label, i.e. the protein conformation near the adenine binding pocket in various ternary complexes, depends on the type of inhibition or substrate employed.

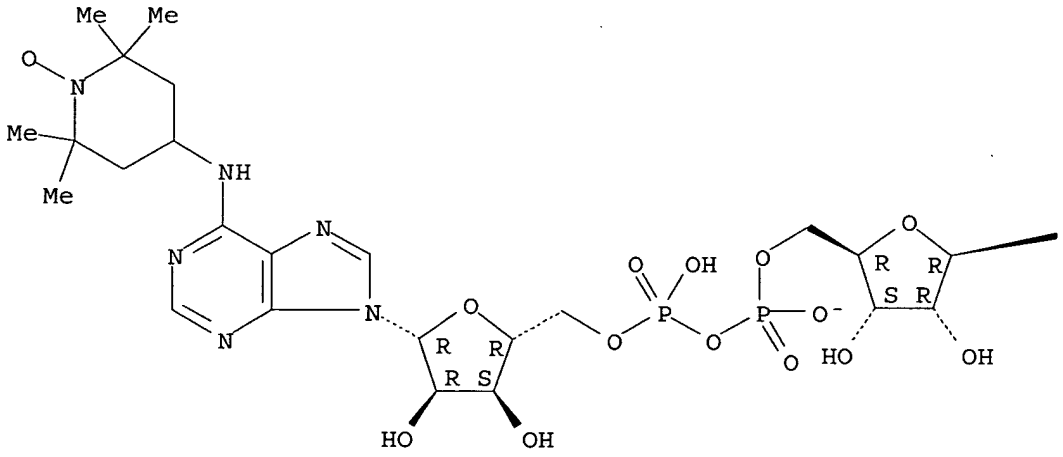
IT **61468-69-7D**, lactate dehydrogenase-inhibitor complexes (formation and properties of)

RN 61468-69-7 HCAPLUS

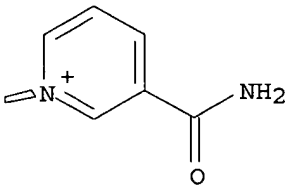
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



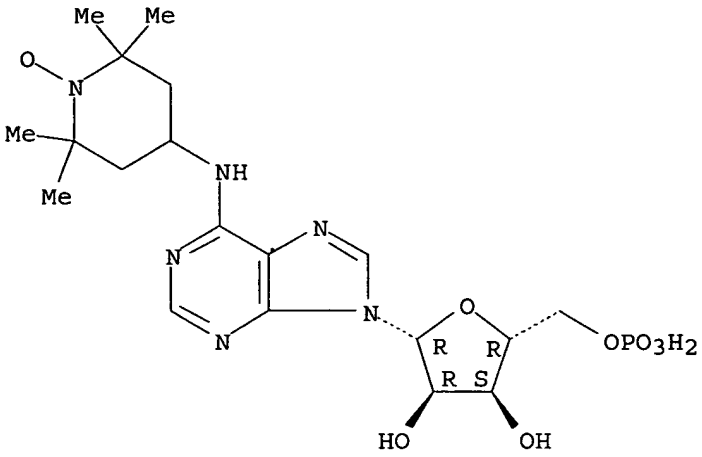
PAGE 1-B



CC 7-3 (Enzymes)
IT 144-62-7D, lactate dehydrogenase-spin labeled NAD complexes
471-47-6D, lactate dehydrogenase-spin labeled NAD complexes
61468-69-7D, lactate dehydrogenase-inhibitor complexes
63958-39-4D, lactate dehydrogenase-inhibitor complexes
(formation and properties of)

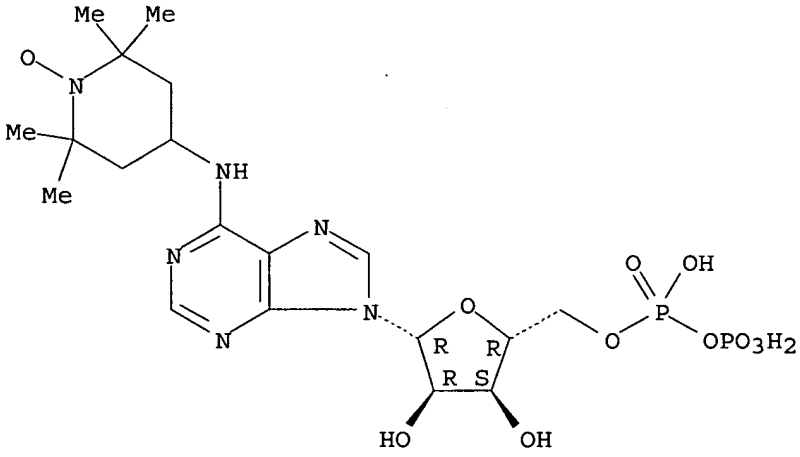
L22 ANSWER 27 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:451766 HCAPLUS
DOCUMENT NUMBER: 91:51766
TITLE: The binding of spin-labeled derivatives of NAD+ and its structural components to pig skeletal muscle lactate dehydrogenase
AUTHOR(S): Deparade, Matthias P.; Trommer, Wolfgang E.
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, 7000/80, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Enzymology (1979), 568(1), 177-82
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In contrast to results previously obtained with the heart muscle lactate dehydrogenase isoenzyme (Wenzel, H.R., et al., 1976), the binding constant of the pig skeletal muscle enzyme for N6-(2,2,6,6-tetramethylpiperidin-4-yl-1-oxyl)-ADP was not significantly greater than that for the corresponding spin-labeled AMP derivative This different behavior can be explained by the substitution of glutamine-31 for alanine in the muscle isoenzyme, which has been proposed to account for the tighter binding of NADH to the heart type. In both isoenzymes the binding of the spin-labeled coenzyme itself is weaker than that found for its structural components, e.g. the ADP and AMP spin-labeled derivs.
IT **54187-54-1 61468-67-5 61468-68-6**
61468-69-7
(lactate dehydrogenase of muscle binding of)
RN 54187-54-1 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

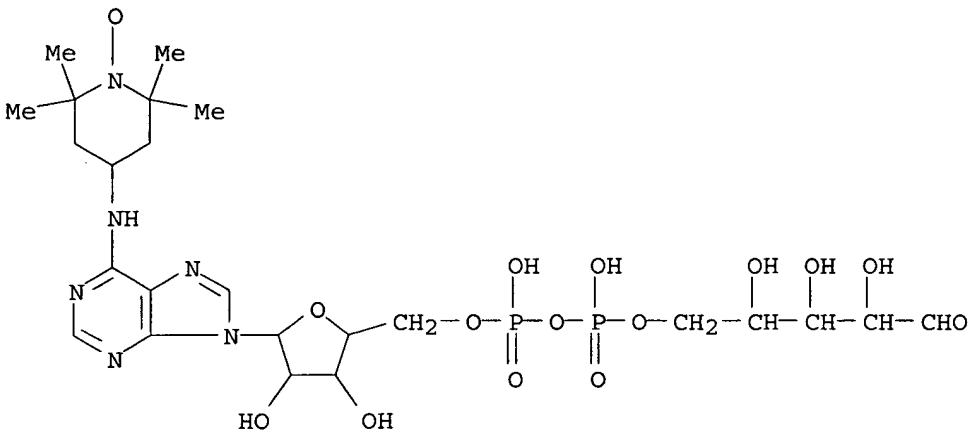


RN 61468-67-5 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



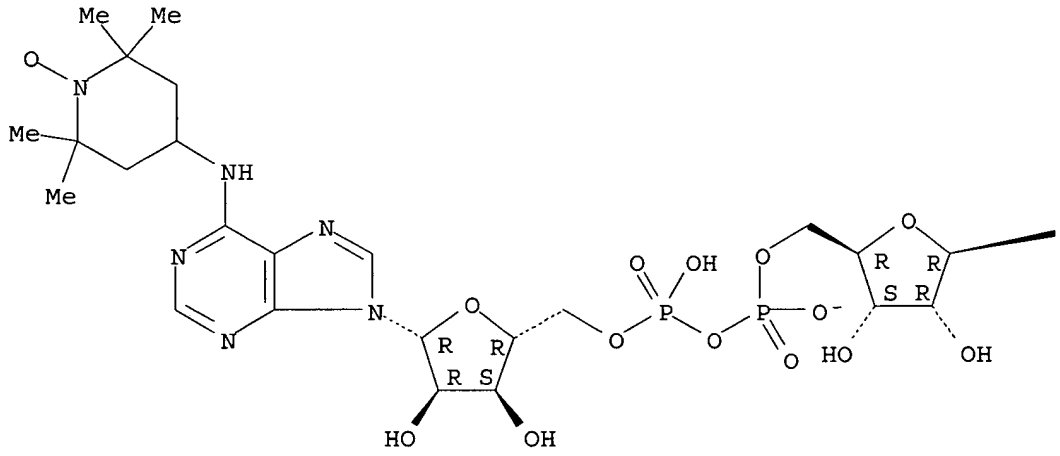
RN 61468-68-6 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5-ester with D-ribose (9CI) (CA INDEX NAME)



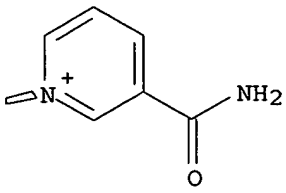
RN 61468-69-7 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



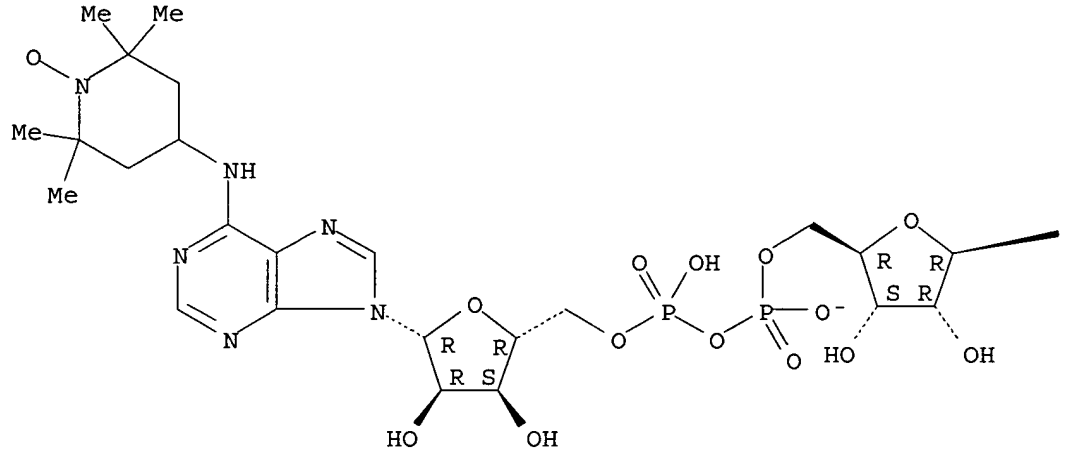
CC 7-3 (Enzymes)
IT **54187-54-1 61468-67-5 61468-68-6**
61468-69-7
(lactate dehydrogenase of muscle binding of)

L22 ANSWER 28 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:163908 HCAPLUS
DOCUMENT NUMBER: 90:163908
TITLE: The nature of the substrate inhibition in lactate dehydrogenases as studied by a spin-labeled derivative of NAD
AUTHOR(S): Trommer, Wolfgang E.; Huth, Helga; Wenzel, Herbert R.
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforschung, Univ. Stuttgart, Stuttgart, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Enzymology (1979), 567(1), 49-59
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The formation of the ternary complex of lactate dehydrogenase from pig heart and skeletal muscle with the adduct of pyruvate to NAD spin-labeled N6 was studied by UV spectroscopy and ESR techniques. According to UV measurements, identical binding characteristics for the natural coenzyme and its spin-labeled analog were found. The rate by which the ESR signal of free spin-labeled NAD decreased upon addition of pyruvate to the binary complexes was substantially different in the 2 isoenzymes. With heart-type isoenzyme, an initial drop followed by a further linear decrease, zero-order in enzyme and coenzyme concentration, was observed In the case of the skeletal muscle isoenzyme, no immediate reaction and a 1st-order process occurred. The initial reaction can be attributed to a noncovalent enzyme-spin-labeled NAD-pyruvate complex with a dissociation constant for pyruvate of 11 mM, thus explaining the well-known substrate inhibition in the heart isoenzyme at concns. >2 mM pyruvate. The further reaction is then determined by the buffer dependent enolization of pyruvate. In the muscle isoenzyme, formation of the covalent adduct is not assisted by prior binding of pyruvate in a noncovalent ternary complex; therefore, the rate depends on the binary complex concentration
IT **61468-69-7**
(ESR of lactate dehydrogenase-bound, pyruvate effect on)
RN 61468-69-7 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-

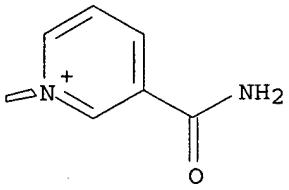
β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
IT **61468-69-7**
(ESR of lactate dehydrogenase-bound, pyruvate effect on)

L22 ANSWER 29 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:148020 HCAPLUS
DOCUMENT NUMBER: 88:148020
TITLE: Conformations of purine ribosyl 5'-nucleotides bound to glycogen phosphorylase b. Nuclear magnetic resonance and electron spin resonance investigations of the effect of substrates
AUTHOR(S): Chachaty, Claude; Forchioni, Alain; Morange, Michel; Buc, Henri
CORPORATE SOURCE: Serv. Chim. Phys., CEN Saclay, Gif-sur-Yvette, Fr.
SOURCE: European Journal of Biochemistry (1978),

82(2), 363-72
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

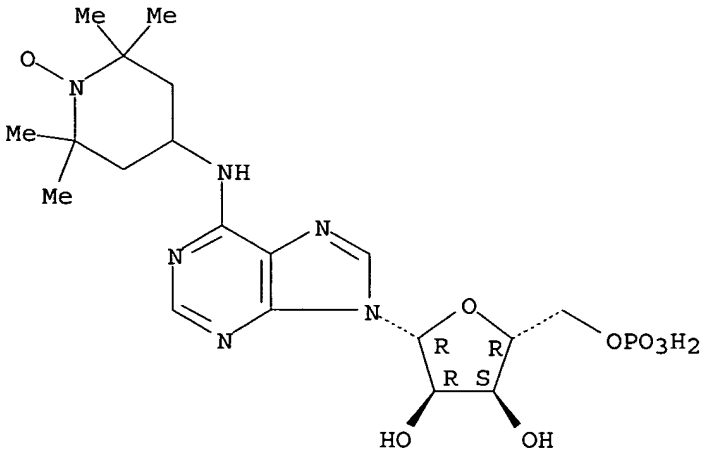
AB The effects of phosphate, glucose 1-phosphate, and glycogen on the binding of several nucleotides to phosphorylase b (I) were investigated by 1H and 2H linewidth measurements and by ESR. A graphical method is proposed to determine the resp. contribution of the strong and weak nucleotide sites of I to the linewidth of H-8, H-2, and H-1'. The contribution of the strong site to the linewidth is governed by the residence time of nucleotides in the case of AMP, 6-chloropurine riboside 5'-monophosphate, and IMP ternary complexes with I and phosphate and by the transverse relaxation time in that of the GMP ternary complex. It is shown that in this latter complex the GMP takes an anti conformation instead of syn conformation in its binary complex with I. This change is related to an enhanced activity of the complex. The reorientation correlation time of binary and ternary complexes estimated from 2H-8 linewidths is of the order of 10-7 s, in agreement with previous 1H linewidth measurements. The dependence of binding of a nucleotide on the concns. of substrates is studied by the ESR of N6-(2,2,6,6-tetramethylpiperidin-4-yl-1-oxy)-AMP. The proton relaxation induced by the nitroxide group of this compound indicates a distance of the order of 1-2 nm between the 2 nucleotide strong sites of I.

IT **54187-54-1**
(ESR of phosphorylase b-bound)

RN 54187-54-1 HCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 7-3 (Enzymes)

IT **54187-54-1**
(ESR of phosphorylase b-bound)

L22 ANSWER 30 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1977:67394 HCAPLUS

DOCUMENT NUMBER: 86:67394

TITLE: Binding studies of a spin-labeled oxidized coenzyme to bovine-liver glutamate

dehydrogenase

AUTHOR(S): Zantema, Alt; Trommer, Wolfgang E.; Wenzel, Herbert; Robillard, George T.

CORPORATE SOURCE: Dep. Phys. Chem., Univ. Groningen, Groningen, Neth.

SOURCE: European Journal of Biochemistry (1977), 72(1), 175-84
CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal

LANGUAGE: English

AB NAD with a nitroxide piperidine ring linked to the NH2 group of the adenine possesses full coenzymic activity with glutamate dehydrogenase. ESR spectra in the presence of glutamate dehydrogenase showed mixts. of free and strongly immobilized spin-label. Binding studies in phosphate buffer demonstrated: (a) weak binary binding to the enzyme with a dissociation constant in the order of 2 mM; (b) an indication for neg. cooperativity or different sites for binding to enzyme-2-oxoglutarate, with dissociation consts. in the order of 20-250 μM; (c) similar but much weaker binding to enzyme-2-oxoglutarate-ADP; (d) and a strong pos. cooperative binding to enzyme-2-oxoglutarate-GTP, dependent on the enzyme concentration Binding of phosphate to the enzyme with a Kd of .apprx.20 mM or binding of pyrophosphate or tripolyphosphate with a Kd of .apprx.2.5 mM enhances the binding of spin-labeled NAD in the presence of 2-oxoglutarate. There is evidence that the binding sites for these phosphates coincide with phosphate binding subsites of GTP.

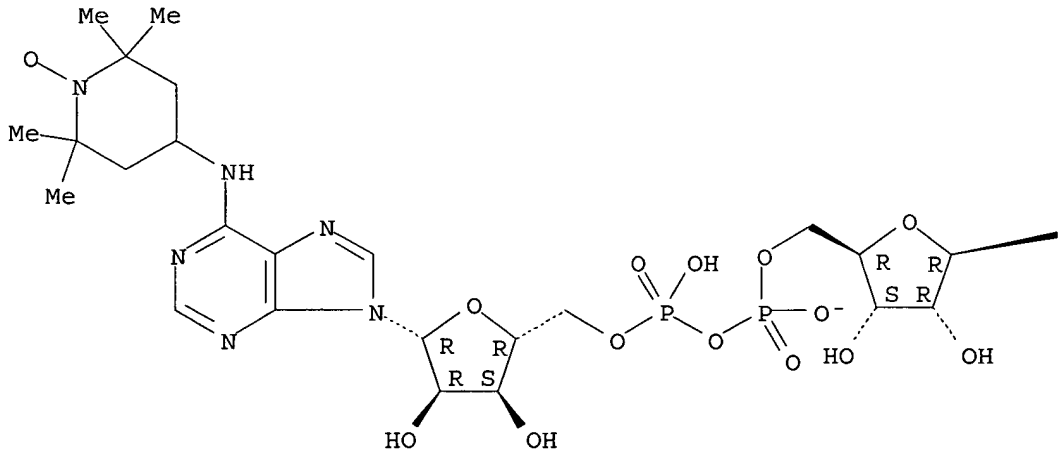
IT **61468-69-7**
(glutamate dehydrogenase binding of)

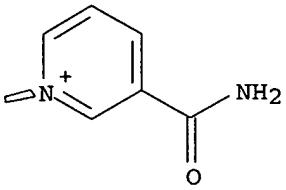
RN 61468-69-7 HCAPLUS

CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

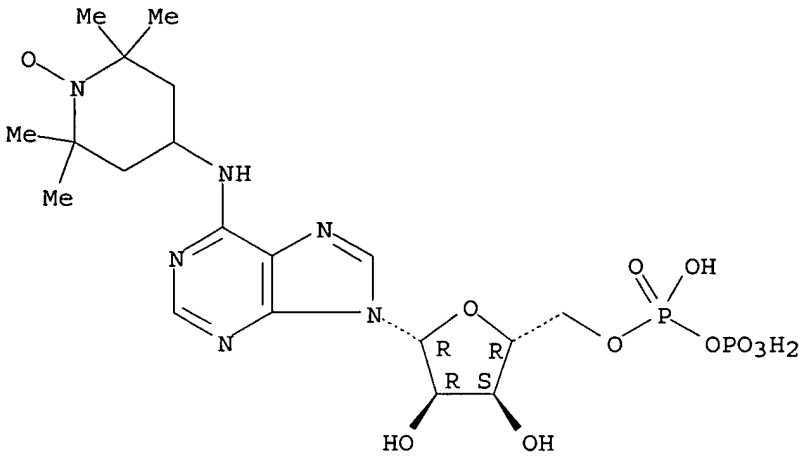




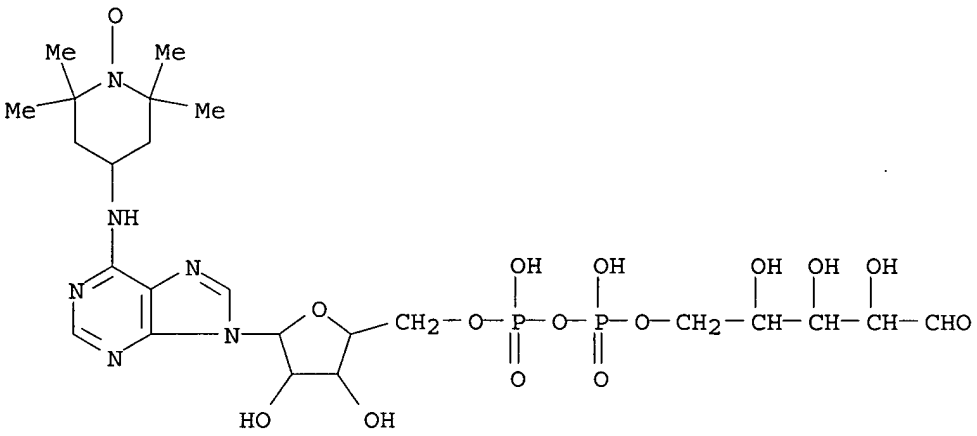
CC 7-3 (Enzymes)
IT **61468-69-7**
(glutamate dehydrogenase binding of)

L22 ANSWER 31 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1977:27216 HCAPLUS
DOCUMENT NUMBER: 86:27216
TITLE: The synthesis of spin-label derivatives of NAD+ and its structural components and their binding to lactate dehydrogenase
AUTHOR(S): Wenzel, Herbert R.; Pfleiderer, Gerhard; Trommer, Wolfgang E.; Paschenda, Klaus; Redhardt, Albrecht
CORPORATE SOURCE: Abt. Chem., Ruhr-Univ. Bochum, Bochum, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta, Enzymology (1976), 452(2), 292-301
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Spin-labeled derivs. of NAD and its structural components [i.e., adenosine, adenine, AMP, ADP, and adenosine 5'-diphosphoribose (ADPR)] were synthesized. Their binding to pig heart lactate dehydrogenase (EC 1.1.1.27) was studied and dissociation consts . were determined The spin-labeled derivs. of ADP and ADPR exhibited a tighter binding than the corresponding NAD derivative This may be attributed to the repulsion of the pos. charged nicotinamide ring by a histidine side chain in the active center of the enzyme.
IT **61468-67-5 61468-68-6 61468-69-7**
(reaction of, with lactate dehydrogenase)
RN 61468-67-5 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



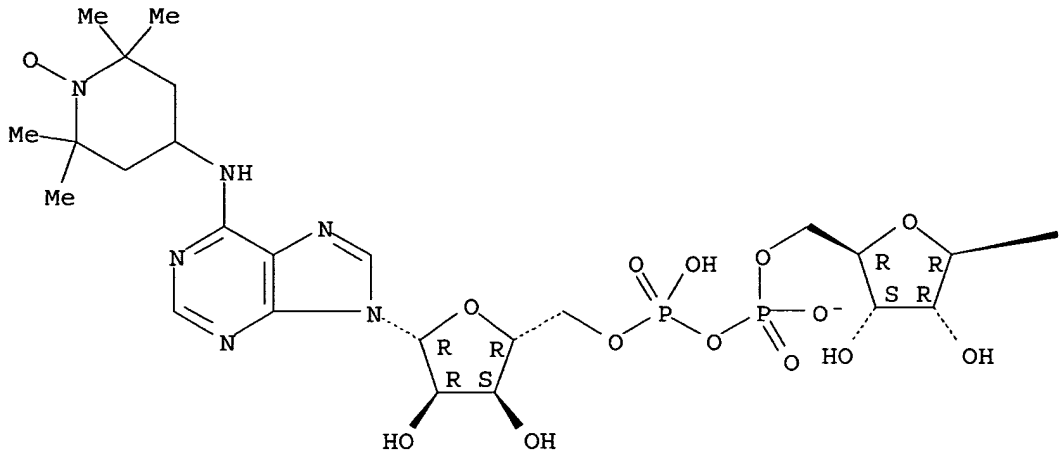
RN 61468-68-6 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5-ester with D-ribose (9CI) (CA INDEX NAME)



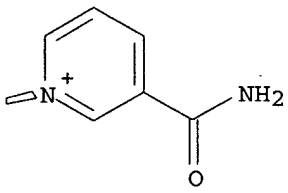
RN 61468-69-7 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 7-3 (Enzymes)
Section cross-reference(s): 33
IT 61468-65-3 61468-66-4 **61468-67-5 61468-68-6 61468-69-7**
(reaction of, with lactate dehydrogenase)

L22 ANSWER 32 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:131992 HCAPLUS
DOCUMENT NUMBER: 84:131992
TITLE: Spin-labelled AMP-an activator of phosphorylase
AUTHOR(S): Busby, Stephen J. W.; Hemminga, Marcus A.; Radda, George K.; Trommer, Wolfgang E.; Wenzel, Herbert
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: European Journal of Biochemistry (1976), 63(1), 33-8
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A spin-labeled AMP derivative and its diamagnetic analog activated

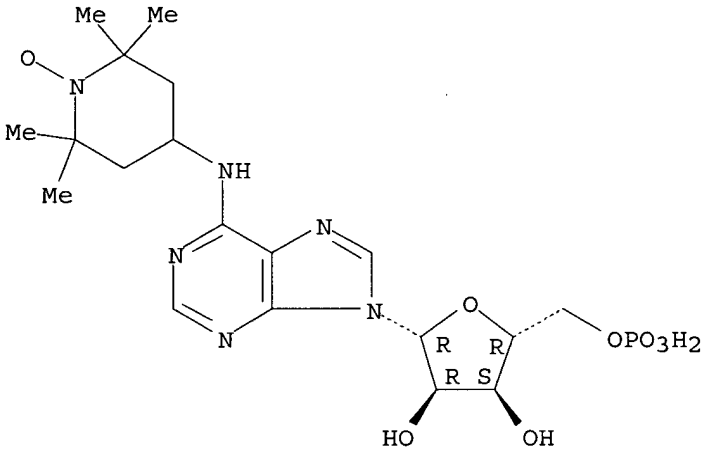
phosphorylase b in the same way, but did not activate phosphorylase a. The ESR spectra of the spin-labeled AMP derivative bound to phosphorylase b and a had powderlike characteristics indicating that the spin label was immobilized on the protein. From changes in the ESR spectrum of spin-labeled AMP as phosphorylase b or a were added, the dissociation consts. were calculated The interactions of spin-labeled AMP and the diamagnetic analog with phosphorylase b and a were monitored by observing changes in the spectral properties of fluorescent and spin-label probes covalently attached to the enzyme. The dissociation consts. of spin-labeled AMP and phosphorylase b or a are 175 ± 25 μM and 15 ± 5 μM, resp. Similar dissociation consts. are obtained for the diamagnetic analog. The effect of these AMP derivs. on the covalently attached probe groups and on phosphorylase activity is compared to the effect of AMP and IMP.

IT **54187-54-1 58933-49-6**
(phosphorylase response to)

RN 54187-54-1 HCAPLUS

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

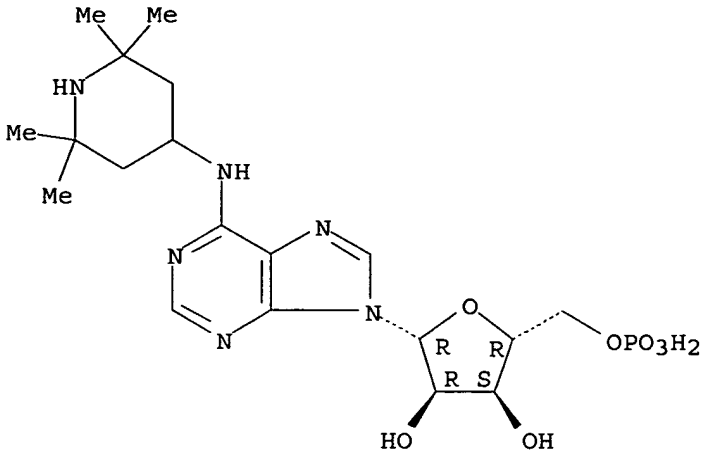
Absolute stereochemistry.



RN 58933-49-6 HCAPLUS

CN 5'-Adenylic acid, N-(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)

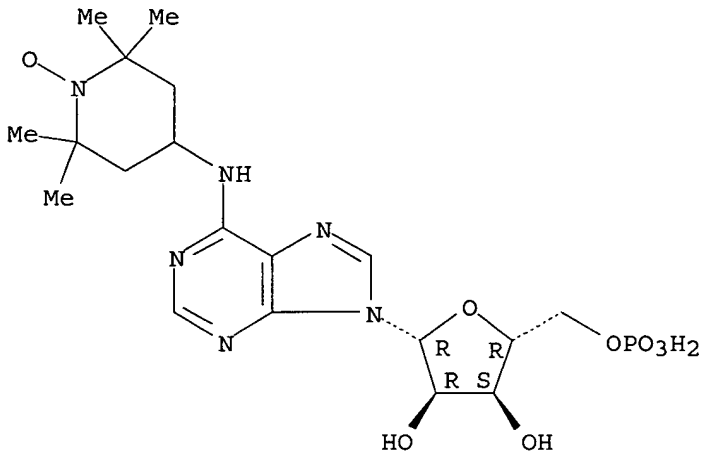
Absolute stereochemistry.



CC 7-5 (Enzymes)
IT **54187-54-1 58933-49-6**
(phosphorylase response to)

L22 ANSWER 33 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:569750 HCAPLUS
DOCUMENT NUMBER: 81:169750
TITLE: Synthesis and biochemical properties of a spin-labeled nicotinamide adenane dinucleotide
AUTHOR(S): Trommer, Wolfgang E.; Wenzel, Herbert; Pfleiderer, Gerhard
CORPORATE SOURCE: Abt. Chem., Univ. Bochum, Bochum, Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (1974), (8), 1357-9
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Reaction of the Ba salt of the acid I (R = OH, R1 = Cl) with 4-amino-2,2,6,6-tetramethyl-1-piperidyloxyl gave the radical I (R = OH, R1 = R3) (II). Condensation of II with nicotinamide mononucleotide gave the spin-labeled nicotinamide adenine dinucleotide I (R = R4, R1 = R3), which functions as coenzyme with various dehydrogenases and can be used for the study of binary and ternary enzyme complexes by the ESR method.
IT **54187-54-1P**
(preparation and reaction with nicotinamide mononucleotide)
RN 54187-54-1 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[9-(5-O-phosphono-β-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

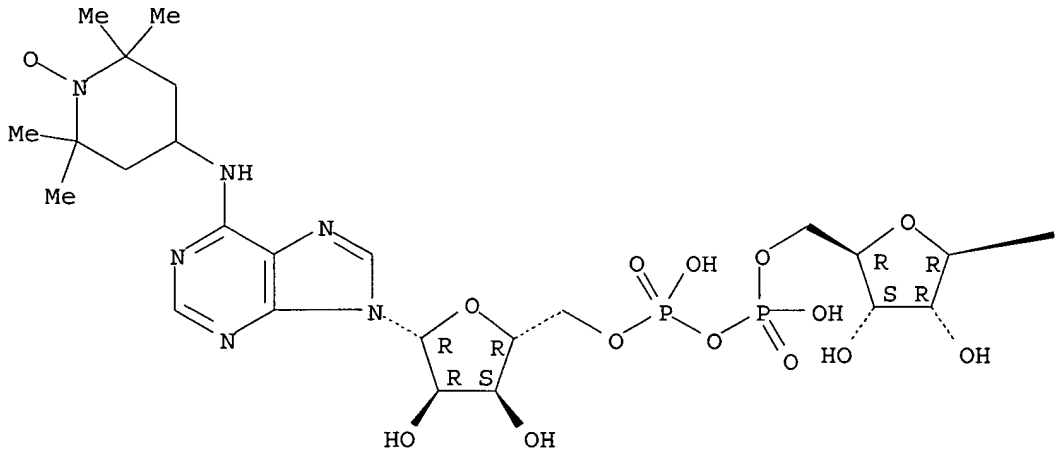
Absolute stereochemistry.



IT **54344-05-7P**
(preparation of)
RN 54344-05-7 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy(phosphonooxy)phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl-, P'→5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, dilithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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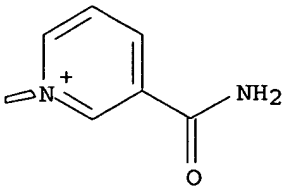
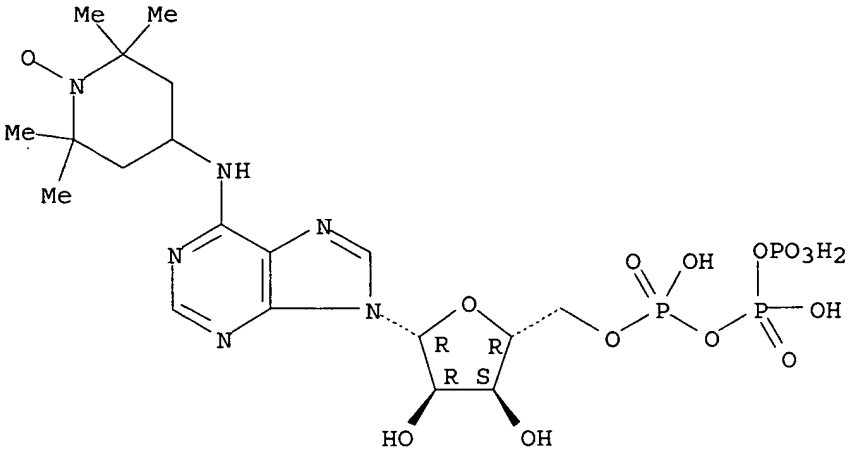


CC 33-7 (Carbohydrates)
IT **54187-54-1P**
(preparation and reaction with nicotinamide mononucleotide)
IT **54344-05-7P**
(preparation of)

L22 ANSWER 34 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:430516 HCAPLUS
DOCUMENT NUMBER: 77:30516
TITLE: Binding of triphosphate spin labels to hemglobin Kempsey
AUTHOR(S): Ogata, Ronald T.; McConnell, Harden M.; Jones, Richard T.
CORPORATE SOURCE: Stauffer Lab. Phys. Chem., Stanford, CA, USA
SOURCE: Biochemical and Biophysical Research Communications (1972), 47(1), 157-65
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The binding of 2,2,6,6-tetramethylpiperidino-1-oxy-4-yl triphosphate (I) to a mutant of human Hb, Hb Kempsey (β-99 Asp → Asn), was studied as a function of heme ligation. The (ligand-free Hb Kempsey)-I complex had a stoichiometry of 1.0 mole of I/mole of Hb Kempsey tetramer and a dissociation constant 1.7 + 10-4 M at 13° in 0.05 M bis-Tris buffer, pH 7.3 and 0.1 M in Cl-. A second spin label, N6-(1-oxyl-2,2,6,6-tetramethyl-4-piperidinyl) adenosine triphosphate, was used to probe the structure of the organic phosphate binding site in ligand-free Hb Kempsey. Neither label binds to fully liganded Hb Kempsey under these conditions. The results of these expts. are consistent with a generalized concerted transition model for cooperative ligand binding to Hb.
IT **33913-54-1**
(reaction of, with Hb Kempsey, ligand binding model in relation to)
RN 33913-54-1 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 6-3 (General Biochemistry)
IT **33913-54-1** 37070-46-5
(reaction of, with Hb Kempsey, ligand binding model in relation to)

L22 ANSWER 35 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1971:445099 HCAPLUS
DOCUMENT NUMBER: 75:45099
TITLE: Proximity of the nucleoside monophosphate and triphosphate binding sites on deoxyribonucleic acid polymerase
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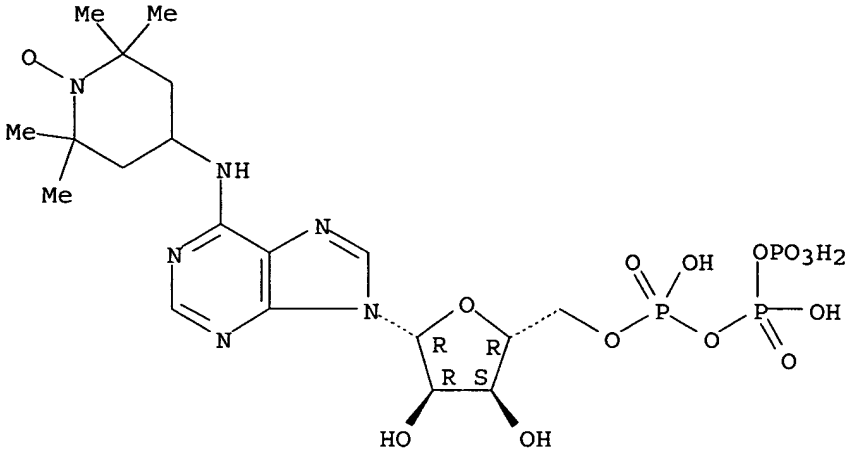
AB The Escherichia coli DNA polymerase exhibits both a deoxyribonucleoside triphosphate binding site and a second site that binds nucleotides that have both a 3'-hydroxyl group in the ribose configuration and a 5'-phosphate linkage. The specificity of the 3'-hydroxyribonucleotide binding site suggested that this site is related to the site that binds the primer terminus of a DNA chain. A paramagnetic analog of ATP was used to bind a spinlabel substrate in the triphosphate binding site. Adenosine 5'-monophosphate was bound in the monophosphate binding site and the NMR relaxation rates of the C2 proton were measured. The separation between the unpaired electron the paramagnetic substrate and the C2 proton of AMP, when both are bound to DNA polymerase, is 7.1 Å. This shows that the two binding sites are adjacent and strongly supports the assertion that the 3'-hydroxy-ribonucleotide binding site is the site that binds the primer terminus of a DNA chain.
IT **33913-54-1**
(reaction of, with deoxyribonucleate nucleotidyltransferase, nucleotide binding sites in relation to)
RN 33913-54-1 HCAPLUS
CN 1-Piperidinyloxy, 4-[[9-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-β-D-ribofuranosyl]-9H-purin-6-yl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 3 (Enzymes)

IT **33913-54-1**
(reaction of, with deoxyribonucleate nucleotidyltransferase, nucleotide binding sites in relation to)